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Vladimir Skliba

TRANSMITTAL LETTER TO THE UNITED STATES DESIGNATED (or ELECTED) OFFICE

Applicant: Andrew Shiau, et al.

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Title of Invention: METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR ACTIVITY

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1. Applicant herewith submits the following items under 35 USC 371 an express request to immediately begin national examination procedures (35 USC 371(f)).

2. Copy of the International application (35 USC 371(c)(2)):

[X] is transmitted herewith.

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Cooley Godward LLP
Attn: Patent Group
Five Palo Alto Square
3000 El Camino Real
Palo Alto, CA 94306-2155
Tel: (650) 843-5000
Fax: (650) 857-0663
MCJ:vla

Respectfully submitted,
COOLEY GODWARD LLP

By: _____
Madison C. Jellins
Reg. No. 35,555

METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR ACTIVITY

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INTRODUCTION

Technical Field

The present invention relates to improved methods and compounds for modulating nuclear receptor activity. In particular, the present invention relates to improved methods and compounds for modulating estrogen receptor activity.

Background

Cells contain receptors that can elicit a biological response by binding various molecules including proteins, hormones and/or drugs. Nuclear receptors represent a super family of proteins that are hormone/ligand-activated transcription factors that enhance or repress transcription in a cell type-, ligand- and promoter-dependent manner. A classic nuclear receptor, the estrogen receptor α (ERα) is a key factor in regulating the differentiation and maintenance of neural, skeletal, cardiovascular and reproductive tissues (Korach, Science 266:1524-1527 (1994); Smith, et al., New Engl. J. Med. 331:1056-1061 (1994)). The nuclear receptor family also includes receptors for glucocorticoids, androgens, mineralocorticoids, progestins, thyroid hormones, vitamin D, retinoids, peroxisome proliferators and eicosanoids. A subset of the nuclear receptor family are the steroid receptors, which include the estrogen, glucocorticoid and progestin receptors.

Overall sequence conservation between nuclear receptors varies between different families of receptors; however, sequence conservation between functional regions, or modules, of the receptors is high. For example, nuclear receptors can be organized into functional modules comprising an N-terminal transcriptional activation domain, a central DNA binding domain (DBD), and a C-terminal ligand binding domain (LBD). The LBD of nuclear receptors represents a hormone/ligand-dependent molecular switch. and recognizes a variety of compounds diverse in their size, shape and chemical properties. Accordingly, the estrogen hormones exert their physiological effects by binding to the estrogen receptor (Beato, et al., Cell

83(6):851-857 (1995); Tsai, et al., Annu. Rev. Biochem. 63:451-86 (1994)). Binding of a hormone to a nuclear receptor's LBD also changes its ability to modulate transcription of DNA, although they may have transcription-independent actions..

All ERα ligands bind exclusively to the C-terminal LBD. Some of these ligands, including the endogenous estrogen, 17β-estradiol (E_2), and the synthetic nonsteroidal estrogen, diethylstilbestrol (DES), function as pure agonists whereas others such as ICI-164,384 function as pure antagonists. Synthetic ligands such as tamoxifen and raloxifene (RAL) belong to a growing class of molecules known as selective estrogen receptor modulators (SERMs), which function as antagonists in specific tissue and promoter contexts (Grese, et al., Proc. Natl. Acad. Sci. USA 94:14105-10 (1997)). The remarkable tissue-specific behavior of tamoxifen was recently demonstrated in a breast cancer prevention trial, reported in Smigel, J. Natl. Cancer Inst. 90:647-8 (1998), where a group of women at high risk for breast cancer who received tamoxifen treatment over a six year period, exhibited an increased incidence of endometrial cancer but a reduced occurrence of certain bone fractures and a dramatic 45% reduction in breast cancer incidence. The rational design of new SERMs and the optimization of existing ones require an understanding of the effects of different ligand chemistries and structures upon ERα transcriptional activity.

Nuclear receptors also bind proteins, such as chaperone complexes, corepressors, or coactivators, that are involved in receptor function. In particular, ligand-dependent activation of transcription by nuclear receptors is mediated by interactions with coactivators. Receptor agonists promote coactivator binding and antagonists block coactivator binding. Hormone binding by a nuclear receptor can increase or decrease binding affinity to these proteins, and can influence or mediate the multiple actions of the nuclear receptors on transcription.

Transcriptional activation by ERα is mediated by at least two separate activation functions (AFs) located within different domains of the protein, AF-1 in the N-terminus, and AF-2 in the LBD. These AFs can act independently or cooperatively, depending on the cell type and the promoter context. The activity of AF-1 is regulated by growth factors acting through the MAP kinase pathway (Kato, et al., Science 270:1491-1494 (1995)) and is generally believed to be activated in a ligand-independent manner, while AF-2 activity ("transcriptional activity") is responsive to ligand binding (Kumar, et al., Cell 51(6):941-951 (1987)). The binding of agonists triggers transcriptional activity whereas the binding of antagonists does not (Berry, et al., EMBO J. 9:2811-8 (1990)). In addition, coactivators mediate transcriptional activity. The structural and

functional nature of the site to which coactivators bind has only recently been defined. Apriletti, et al., US Provisional No. 60/079,956, filed March 30, 1998, the disclosure of which is incorporated herein by reference.

Recent structural studies suggest that ligands regulate transcriptional activity by directly affecting the structure of the LBD. Comparison of the structure of the unliganded human retinoid X receptor α LBD (Bourguet, et al., Nature 375:377-82 (1995)) with the structures of the liganded LBDs of the human retinoic acid receptor γ (RARγ) (Renaud, et al., Nature 378:681-689 (1995) and Wurtz, et al., Nat. Struct. Biol. 3:87-94(1996)), the thyroid hormone receptor α (TRα) (Wagner, et al., Nature 378:690-697 (1995)), the progesterone receptor (Williams, et al., Nature 393:392-395 (1998)) and the ERα (Brzozowski, et al., Nature 389:753-758 (1997); Tanenbaum, et al., Proc. Natl. Acad. Sci. USA 95:5998-6003 (1998)) suggests that an agonist-induced conformational change involving the repositioning of helix 12, the most C-terminal helix of the LBD, is essential for transcriptional activity. Because certain point mutations in helices 3, 5 and 12 abolish transcriptional activity but have no effect on ligand or DNA binding, these regions of the LBD have been predicted to form part of a recognition surface, created in the presence of agonist, for molecules that link the receptor to the general transcriptional machinery (Danielian, et al., EMBO J. 11:1025-33(1992); Feng, et al., Science 280:1747-9 (1998); Henttu, et al., Mol. Cell. Biol. 17:1832-9 (1997); Wrenn, et al., J. Biol. Chem. 268:24089-24098 (1993)). The structures of the LBD complexed with E_2 and RAL show that although both ligands bind at the same site within the core of the LBD (Brzozowski, et al., supra), each of these ligands induces a different conformation of helix 12. Whereas helix 12 in the E_2-LBD complex packs against the helices 3, 5/6 and 11 in a conformation that has been observed for the corresponding helix in other agonist-bound NR LBD structures, helix 12 in the RAL-LBD complex is bound in a hydrophobic groove composed of residues from helices 3 and 5. This alternative orientation of helix 12 partially buries residues in the groove that are necessary for transcriptional activity, suggesting that RAL and possibly other antagonists block transcriptional activity by disrupting the topography of the coactivator binding site surface.

Biochemical and genetic approaches have led to the identification of several proteins that associate in a ligand-dependent manner with ERα (Horwitz, et al., Mol. Endocrinol. 10:1167-1177 (1996)) including SRC-1/N-CoA1 (Onate, et al., Science 270:1354-1357 (1995)), GRIP1/TIF2/SRC-2 (Hong, et al., Proc. Natl. Acad. Sci. USA 93(10):4948-4952 (1996) and Voegel, et al. EMBO J. 15:3667-3675 (1996)), p/CIP/RAC3/ACTR/AIB1/SRC-3 (Anzick, et al.,

Science 277:965-968(1997), Chen, et al., Cell 90(3):569-80 (1997), Li, et al., Proc. Natl. Acad. Sci. USA 94:8479-84 (1997) and Torchia, et al., Nature 387:677-684 (1997)) and CBP/p300 (Hanstein, et al., Proc. Natl. Acad. Sci. USA 93:11540-11545 (1996)). These proteins have been classified as transcriptional coactivators because they enhance ligand-dependent transcriptional activation by ERα as well as by several other NRs (Glass, et al., Curr. Opin. Cell Biol. 9:222-32 (1997); Torchia, et al., supra). The observation of partial hormone resistance in mice with a disrupted SRC-1 gene (Xu, et al., Science 279:1922-1925(1998)) provides compelling evidence that coactivators are required for NR function *in vivo*. Consistent with its proposed role in AF-2 directed transcriptional activation, SRC-1 possesses histone acetylase activity and the ability to interact not only with agonist-bound receptors but also with other coactivators and several general transcription factors (Kamei, et al., Cell 85(3):403-14 (1996); Onate, et al., supra; Spencer, et al., Nature 389:194-8 (1997); Takeshita, et al., Endocrinology 137:3594-7 (1996)). SRC-1 and GRIP1 also bind to the agonist-bound LBDs of both the human TRβ and human ERα using the putative coactivator binding site (Feng, et al., supra).

Members of the p160 family of coactivators such as SRC-1, GRIP1/TIF2/SRC-2, and p/CIP/RAC3/ACTR/AIB1/SRC-3 as well as other coactivators recognize agonist-bound NR LBDs through a short signature sequence motif, LXXLL (SEQ ID NO:1) (where L is leucine and X is any amino acid), known as the NR box (Ding, et al., Mol. Endocrinol. 12:302-313 (1998); Heery, et al., Nature 387:733-736 (1997); Le Douarin, et al., EMBO J. 15:6701-15 (1996); Torchia, et al., supra). Mutagenesis studies indicate that the affinity of coactivators for NR LBDs is determined principally, if not exclusively, by these NR boxes (Ding, et al., supra); Heery, et al., Nature 387:733-736 (1997); Le Douarin, et al., EMBO J. 15:6701-15 (1996); Torchia, et al., supra). Each of the p160 coactivators contains several NR boxes. The NR boxes within SRC-1, GRIP1 and TIF2 have been demonstrated to recognize different NRs with different affinities (Ding, et al., supra; Kalkhoven, et al., EMBO J. 17:232-43 (1998); Voegel, et al., EMBO J. 17:507-19 (1998)), but the reasons for these binding preferences are unknown.

Darimont, et al., "Structure and specificity of nuclear receptor-coactivator interactions" Genes Dev. 12:3343-3356 (1998) describes structural studies of the complex between TRβ and the GRIP1 NR Box II peptide and biochemical studies of GRIP1 binding to TRβ and GR. The PPARγ/SRC-1 peptide complex is described in Nolte, et al., Nature 395:137-143 (1998).

The medical importance of nuclear receptors is significant. They have been implicated in breast cancer, prostate cancer, cardiac arrhythmia, infertility, osteoporosis, hyperthyroidism,

hypercholesterolemia, obesity and other conditions. For example, compounds that modulate ERα transcriptional activity are currently being used to treat osteoporosis, cardiovascular disease and breast cancer (Gradishar, et al., J. Clin. Oncol. 15:840-52 (1997) and Jordan, J. Natl. Cancer Inst. 90:967-71 (1998)).

A need continues to exist for further identification and characterization of the key residues within the ligand binding domains of the nuclear receptors, and molecules that affect the receptor by binding to these sites. Understanding these interactions provides a basis for iterative drug design, synthesis, and selection. It also would be advantageous to devise methods and compositions for reducing the time required to discover compounds that target these binding sites and administer them to organisms to modulate physiological processes regulated by the nuclear receptors, and the estrogen receptor in particular.

SUMMARY OF THE INVENTION

The present invention relates to the further identification and manipulation of the ligand binding domain (LBD) of nuclear receptors, which facilitates the design of compounds that bind to the LBD and modulate nuclear receptor activity, and the estrogen receptor in particular. The compounds include agonists and antagonists that modulate nuclear receptor activity, and can be receptor-, cell- and/or tissue-specific. In particular, the compounds modulate nuclear receptor activity by affecting coactivator-coactivator binding site interactions.

The present invention also includes protein cocrystals of the nuclear receptors with an agonist bound to the LBD and a peptide bound to the coactivator binding site and methods for making them. Similarly, the invention also includes protein cocrystals of the nuclear receptors with an antagonist bound to the LBD and methods for making them. The cocrystals provide means to obtain atomic modeling information of the specific amino acids and their atoms forming the LBD and coactivator binding sites and that interact with molecules that bind to the sites. The cocrystals also provide modeling information regarding the ligand:nuclear receptor and coactivator:nuclear receptor interactions, as well the structure of ligands bound thereto.

The present invention further provides methods for identifying and designing molecules that modulate ligand binding to a nuclear receptor using atomic models of nuclear receptors. The method involves modeling test compounds that fit spacially into a nuclear receptor LBD using an atomic structural model comprising a nuclear receptor LBD or portion thereof, screening the test compounds in an assay, such as a biological assay, characterized by binding of

a test compound to the nuclear receptor LBD, and identifying a test compound that modulates ligand binding to the receptor.

The invention also includes compositions and methods for identifying key residues within the LBDs of nuclear receptors. The methods involve examining the surface of a nuclear receptor of interest to identify residues that modulate ligand and/or coactivator binding. The residues can be identified by homology to the key residues within the LBD of human ERα described herein. Overlays and superpositioning with a three dimensional model of a nuclear receptor's LBD, and/or a portion thereof, also can be used for this purpose. Additionally, alignment and/or modeling can be used as a guide for the placement of mutations on the LBD surface to characterize the nature of the site in the context of a cell.

Also provided is a method of modulating the activity of a nuclear receptor. The method can be *in vitro* or *in vivo*. The method comprises administering *in vitro* or *in vivo* a sufficient amount of a compound that binds to the ligand binding domain and acts either as an agonist or an antagonist. Preferred compounds bind to the site with greater affinity than ligands found in a cell of interest.

The invention further includes a method for identifying an agonist or antagonist of ligand binding to a nuclear receptor. The method comprises providing the atomic coordinates comprising a nuclear receptor ligand binding domain or portion thereof to a computerized modeling system; modeling compounds which fit spatially into the nuclear receptor ligand binding domain; and identifying in an assay, for example a biological assay, for nuclear receptor activity a compound that increases or decreases activity of the nuclear receptor through binding the ligand binding domain.

Also provided is a machine-readable data storage medium with information for constructing and manipulating an atomic model comprising the ligand binding domain or portions thereof. The medium comprises a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex for a nuclear receptor ligand binding domain.

Also provided is a method of identifying a compound that selectively modulates the activity of one type of nuclear receptor compared to other nuclear receptors. The method is exemplified by modeling test compounds that fit spatially and preferentially into a nuclear receptor ligand binding domain of interest using an atomic structural model of a nuclear receptor

LBD. selecting a compound that interacts with one or more residues of the LBD unique in the context of that site. and identifying in an assay, for example a biological assay, for ligand binding activity a compound that selectively binds to the LBD compared to other nuclear receptors. The unique features involved in receptor-selective ligand binding can be identified by comparing atomic models of different nuclear receptors or isoforms of the same type of receptor.

The invention finds use in the selection and characterization of peptide. peptidomimetic. as well as other compounds, such as small organic molecules, identified by the methods of the invention, particularly new lead compounds useful in treating nuclear receptor-based disorders, in particular steroid receptor-based disorders, and more specifically estrogen receptor-based disorders.

BRIEF DESCRIPTION OF THE DRAWINGS

Figure 1 provides a stereo view of the electron density of the complexes, where Figure 1A is a stereo view of the electron density of the DES-ERα LBD-GRIP1 NR Box II peptide complex and Figure 1B is a stereo view of the electron density of the OHT-ERα LBD complex. Figure 1 is a black and white graphical representation of a figure that was generated using BOBSCRIPT (Esnouf, J. Mol. Graph. Model. 15, 132-4, 112-3 (1997)) and rendered using Raster3D (Merritt, et al., Acta Crystallogr. D 50:869-873 (1994)).

Figure 2 was generated using BOBSCRIPT and rendered using Raster3D as described above. Figure 2A shows the overall structure of the DES-ERα LBD-GRIP1 NR Box II peptide complex in two orthogonal views. Figure 2B shows the overall structure of the OHT-ERα LBD complex in two orthogonal views similar to those of the agonist complex in Figure 2A.

Figures 3A and 3B were generated using BOBSCRIPT and rendered using Raster3D as described above. Figures 3C and 3D were created using GRASP (Nicholls. GRASP Manual (New York: Columbia University, 1992)). Figure 3A shows a close-up view of the coactivator peptide bound to the LBD, i.e., the NR Box II peptide/LBD interface. The regions of the LBD that do not interact with the peptide have been omitted for clarity. Helices 3. 4 and 5 are labeled H3, H4 and H5 respectively. The side chains of receptor residues which interact with the peptide are depicted. except for Lys 362 (blue) and Glu 542 (red), the side chains are colored by atom type (carbon and sulfur atoms are colored green. oxygen atoms are colored red and nitrogen atoms are colored blue). Helix 12 is colored magenta. The peptide. colored gold. is depicted as a Cα worm; only the side chains of Ile 689 and the three motif leucines (Leu 690. Leu 693 and Leu 694) are drawn (Figure 3C). Figure 3B shows the helix 12/LBD interface as a close-up view

of the OHT-LBD complex showing helix 12 bound to part of the coactivator binding site. Only the side chains of residues that interact with helix 12 are drawn (with the exception of side chain of His 373 which is omitted for clarity). Except for Lys 362 (blue) and Glu 380 (red), the side chains are colored by atom type as specified for Figure 3A. Residues 530-551 are depicted as a Cα worm; residues 536-544 are colored magenta. The side chains of Leu 536, Tyr 537, Leu 540, Met 543 and Leu 544 are shown. Figure 3C is a molecular surface representation showing the electrostatic surface of the ERα LBD bound to the NR Box II peptide as positive (blue) and negative (red) regions, as calculated in GRASP. The coactivator peptide is depicted as in Figure 3A and the view is equivalent to that in Figure 3A. The side chains of Leu 690 and Leu 694 are bound in a hydrophobic groove and those of Ile 689 and Leu 693 rest against the edge of this groove. Figure 3D shows the electrostatic surface of the ERα LBD complexed with OHT, showing positive (blue) and negative (red) regions as in Figure 3C. Residues 530-511 are depicted as in Figure 3B and the view is equivalent to that in Figure 3B. Whereas the side chains of Leu 540 and Leu 544 are embedded in the hydrophobic groove, that of Met 543 lies along the edge of this groove.

Figure 4 was generated using LIGPLOT (Wallace, et al., Protein Eng. 8:127-34 (1995)) and provides schematic diagrams illustrating the DES interactions with the LBD (Figure 4A) and OHT interactions with the ligand binding pocket (Figure 4B). Residues that interact with the ligands are drawn at approximately their true positions. The residues that form van der Waals contacts with ligand are depicted as labeled arcs with radial spokes that face towards the ligand atoms with which they interact. The residues that hydrogen bond to ligand are shown in ball-and-stick representation. Hydrogen bonds are represented as dashed cyan lines and the distance of each bond is given. The ligand rings and the individual ligand atoms are labeled.

Figure 5 was generated using BOBSCRIPT and rendered using Raster3D as described above, and shows a comparison of helix 12 from the OHT complex and the NR Box II peptide. Figure 5A and Figure 5B are stereo views. The structures of the OHT-LBD complex and the DES-LBD-NR Box II peptide complex were overlapped using the Cα coordinates of residues 306-526 of the LBD. Helix 12 from the DES-LBD-coactivator peptide complex is omitted for clarity. Residues 536-551 (helix 12=residues 536-544) from the OHT-LBD complex are colored magenta and the peptide is colored gold. The hydrogen bonds between the ε-amino group of Lys 362 and the backbone carbonyls of residues 543 and 544 of helix 12 are illustrated as dashed magenta lines. The hydrogen bonds between the ε-amino group of Lys 362 and the backbone

carbonyls of residues 693 and 696 of the coactivator peptide are depicted as dashed orange lines. The following abbreviations are used on helix 12: L540=Leu 540, M543=Met 543, and L544=Leu 544. The following abbreviations are used on the peptide: L690=Leu 690, L693=Leu 693 and L694=Leu 694.

Figures 6A and 6D were generated using BOBSCRIPT and rendered using Raster3D as described above. Figures 6B and 6C were created using MidasPlus (Huang, et al., J. Mol. Graph. 9:230-6, 242 (1991)). Figure 6A shows that agonists and antagonists promote different LBD conformations, as ribbon representations of the DES complex (without the coactivator peptide), the OHT complex and the E_2 complex such as is described in Tanenbaum, et al., supra. The hormones are shown in space-filling representation. In each complex, helix 12 is colored magenta and the main chain of residues 339 to 341, 421 to 423, and 527 to 530 is indicated in red. Helices 3, 8 and 11 (H3, H8 and H11 respectively) are labeled in the DES complex. Figure 6B shows DES bound in the ligand binding cavity. A cross-section of a space-filling model of the LBD bound to DES (green) showing the ligand completely embedded in the ligand binding cavity. The A' ring of DES (A'), Phe 404 (404), Met 421 (421) and Phe 425 (425) are labeled. The carbon atoms of side chain of Met 421 are colored magenta, and the sulfur atom is colored yellow. Figure 6C is a cross-section of a space-filling model of OHT (red) bound in the ligand binding pocket. The view is equivalent to that in Figure 6B. The B ring of OHT (B), Phe 404 (404), Met 421 (421) and Phe 425 (425) are labeled. The side chain of Met 421 is colored as in Figure 6B. The conformation of the B ring forces Met 421 to adopt a different conformation than in the one it adopts in the DES complex (compare with Figure 6B). Figure 6D provides a comparison of the ligand binding pocket bound to DES (green) and to OHT (red). The structures of the OHT complex and the DES complex were overlapped as in Figure 5. The A rings of both ligands point out of the page; the B ring of OHT and the A' ring of DES point into the page. The LBD bound to OHT is colored blue and the LBD bound to DES is colored light blue-grey. The side chains of some of the residues whose conformations are dramatically different between the two complexes are drawn; Met 342 (342), Met 343 (343), Phe 404 (404), Met 421 (421), Ile 424 (424), Phe 425 (425), His 524 (524), Leu 525 (525), Met 528 (528). The sulfur atom of Met 421 is colored yellow in both structures.

Figure 7 illustrates a model of antagonist action. Agonist (white triangle) binding stabilizes a conformation of the LBD that promotes coactivator (yellow) binding. Residues 527-530 (red) are part of helix 11 (blue) and the length of the interhelical loop prevents helix 12

(magenta) from binding to the static region of the surface involved in transcriptional activity. Antagonist (white cross) side chains preclude helix 12 from being positioned over the ligand binding pocket. Residues 527-530 (red) adopt an extended conformation as a result of antagonist-driven structural perturbations in and around the ligand binding pocket. The length of the loop between helices 11 and 12 allows helix 12 to bind the static region of this surface and inhibit coactivator recognition.

Figure 8 shows alignment of amino acid sequences (single letter amino acid designations) containing residues that form the coactivator binding sites of several nuclear receptors: human and recombinant thyroid hormones (hTRβ and rTRα) (SEQ ID NO:5 and 6 and SEQ ID NO:7 and 8), retinoids (hRARγ and hRXRα) (SEQ ID NO:9 and 10 and SEQ ID NO:11 and 12), peroxisome (hPPARγ) (SEQ ID NO:13 and 14), vitamin D (hVDR) (SEQ ID NO:15 and 16), estrogen (hERα) (SEQ ID NO:17 and 18), glucocorticoid (hGR) (SEQ ID NO:19 and 20), progestin (hPR) (SEQ ID NO:21 and 22), mineralocorticoid (hMR) (SEQ ID NO:23 and 24) and androgen (hAR) (SEQ ID NO:25 and 26). The boxes represent residues of alpha-helix (H3, H4, H5, H6 and H12); lower case letters "h" and "q" represent hydrophobic and polar residues, respectively. The numbered positions at the top of the table, 280, 281, etc., correspond to hTRβ residues.

DESCRIPTION OF SPECIFIC EMBODIMENTS

The present invention provides methods and compositions for identifying compounds that modulate nuclear receptor activity, in particular steroid receptor activity, and more particularly estrogen receptor activity. The compounds are nuclear receptor agonists or antagonists that bind to the ligand binding domain. Compounds that bind to the LBD also are provided. The compounds can be natural or synthetic. Preferred compounds are small organic molecules, peptides and peptidomimetics (e.g., cyclic peptides, peptide analogs, or constrained peptides).

Certain residues within the ERα LBD have been identified that are of particular importance:Met343, Leu346, Ala350, Glu353, Leu384, Leu387, Leu391, Arg394, Phe404, Met421, Leu428, Gly521, His524, Leu525 and Met528 (See Figure 4A). Of these, some have been found to directly or indirectly effect the positioning of helix 12: Met343, Met421, His524, Leu525 and Met528. Interactions with these particular residues, such as occurs when DES binds to the receptor stabilizes a conformation of the LBD that promotes coactivator binding. Modifications to a ligand that enhance binding or interaction with these residues would provide

for an improved agonist of receptor activity. Similarly, modifications to a ligand that adversely affects the binding or interaction with these residues would provide for an improved antagonist.

In addition, it is believed that the ERα Tyr537 residue plays a role in stabilizing the unliganded receptor so that helix 12 is free to interact with the coactivator binding site. The ER is quite unique in having a tyrosine at this position as hTRβ, rTRα, hRARγ, hGR, hPR, hMR and hAR all have a proline residue. hRXRα has as aspartic acid residue, hPPARγ has a histidine residue and hVDR has a threonine residue at positions corresponding to the Tyr 537 residue of hERα. Therefore, selective agonists and antagonists can be designed for the estrogen receptor that interact with Tyr 537.

Traditional antagonists such as OHT or RAL have side chains that directly block helix 12 positioning as it is in the agonist complexes (DES or E_2). In addition, it is expected that ligand-induced perturbations are required to allow helix 12 to reach into the coactivator helix binding site, thereby blocking coactivator binding and inhibiting transcriptional activity. Such perturbations or interference with proper interactions with one or more of these LBD residues, has been found to relax the receptor, disassembling the receptor's secondary structure and resulting in unwinding of helix 11. The unwinding of helix 11 increases the length of the loop between helices 11 and 12, allowing helix 12 to move away from the ligand binding pocket and towards the coactivator binding site, where it occludes the coactivator recognition groove by mimicking the interactions of the coactivator, and thus inhibits coactivator recognition (see Figure 7). Modifications to a ligand that interfere with binding or interaction with one or more of the amino acids positions indicated, would cause receptor relaxation, affecting the receptor's secondary structure and cause the unwinding of helix 12. Compounds based upon such modified ligands would act as antagonists.

Accordingly, one aspect of the invention is a method of identifying a compound that modulates (i.e., increases or decreases) nuclear receptor activity, comprising: modeling test compounds that fit spatially into a nuclear receptor ligand binding domain of interest using an atomic structural model of the estrogen receptor α ligand binding domain or portion thereof, screening the test compounds in an assay, for example a biological assay, characterized by binding of a test compound to the ligand binding domain, and identifying a test compound that modulates nuclear receptor activity, wherein the atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human estrogen receptor α Met343, Leu346, Ala350, Glu353, Leu384, Leu387, Leu391, Arg394, Phe404, Met421, Leu428,

Gly521, His524, Leu525 and Met528, preferably Met343, Met421, His524, Leu525 and Met528. In a preferred embodiment, the nuclear receptor is the ER. The test compound can be an agonist and nuclear receptor activity is measured by binding of a coactivator or a compound that mimics a coactivator, to the coactivator binding site, as defined below. On the other hand, the test compound can be an antagonist and nuclear receptor activity is measured by the unwinding of helix 12 and/or the blocking of coactivator binding to the coactivator binding site. The screening is typically *in vitro*, and high throughput screening is preferable. Suitable test compounds can be designed, as is described later, or can be obtained from a library of compounds, and include, by means of illustration and not limitation, small organic molecules, peptides and peptidomimetics. The method described above may also include the step of providing the atomic coordinates of the estrogen receptor α ligand binding domain or portion thereof to a computerized modeling system, prior to said modeling step.

As used herein, the term "portion thereof" is intended to mean the atomic coordinates corresponding to a sufficient number of residues or their atoms of the LBD that interact with a compound capable of binding to the site. This includes receptor residues having an atom within 4.5Å of a bound compound or fragment thereof. Thus, for example, the atomic coordinates provided to the modeling system can contain atoms of the nuclear receptor LBD, part of the LBD such as atoms corresponding to the LBD or a subset of atoms useful in the modeling and design of compounds that bind to a LBD.

The atomic coordinates of a compound that fits into the ligand binding domain also can be used for modeling to identify compounds or fragments that bind the site. By "modeling" is intended quantitative and qualitative analysis of molecular structure/function based on atomic structural information and receptor-ligand agonists/antagonists interaction models. This includes conventional numeric-based molecular dynamic and energy minimization models, interactive computer graphic models, modified molecular mechanics models, distance geometry and other structure-based constraint models. Modeling is preferably performed using a computer and may be further optimized using known methods. By "fits spatially" is intended that the three-dimensional structure of a compound is accommodated geometrically by a cavity or pocket of a nuclear receptor LBD.

It is expected that targeting the corresponding amino acids on other nuclear receptors will have the same effect. Accordingly, one embodiment of the invention pertains to methods of designing antagonists that bind the LBD of a nuclear receptor but do not interact with one of

more residues within the LBD that correspond to (i.e., the same as or equivalent to) human ERα residues Met343, Leu346, Ala350, Glu353, Leu384, Leu387, Leu391, Arg394, Phe404, Met421, Leu428, Gly521, His524, Leu525 and Met528, preferably Met343, Met421, His524, Leu525 and Met528. Similarly, another embodiment of the invention pertains to methods of designing agonists that bind the LBD of a nuclear receptor and have enhanced interaction with one or more residues within the LBD that correspond to the human ERα residues Met343, Leu346, Ala350, Glu353, Leu384, Leu387, Leu391, Arg394, Phe404, Met421, Leu428, Gly521, His524, Leu525 and Met528, preferably Met343, Met421, His524, Leu525 and Met528. An example of enhanced interaction is where the agonist has a greater binding affinity for one or more of said residues, as compared to an endogenous ligand. Such corresponding positions for other members of the nuclear receptor family are shown in Table 1, which provides an alignment of amino acid sequences (one letter amino acid designations) containing residues from the ligand binding domains of several nuclear receptors that correspond to the designated positions on the human estrogen receptor (hERα): recombinant thyroid hormone (rTRα), retinoids (hRARγ and hRXRα), glucocorticoid (hGRα), progestin (hPR), mineralocorticoid (hMR) and androgen (hARα). It is understood that Table 1 is merely illustrative of the invention and is not intended to be limiting in any manner. Accordingly, it is understood that corresponding amino acid residues of other nuclear receptors such as other estrogen receptors, thyroid receptors, retinoid receptors, glucocorticoid receptors, progestin receptors, mineralocorticoid receptors, androgen receptors, peroxisome receptors and vitamin D receptors, may also be used in the methods of the invention.

Table 1

hERα	M343	M421	F425	H524	L525	M528
hPR	L715	F794	I798	Y890	C891	T894
hARα	L701	M780	Q784	F876	T877	L881
hGRα	M560	M639	Q643	Y735	C736	T740
hMR	L766	M845	L849	F941	C942	T946
hRARγ	W227	F304	L308	R396	A397	L401
hRXRα	V265	G343	F346	H435	L436	F440
rTRα	F215	L292	V296	R384	F385	M389

The term "coactivator binding site" is used herein to mean a structural segment or segments of the nuclear receptor polypeptide chain folded in such a way so as to give the proper geometry and amino acid residue conformation for binding coactivator. This is the physical arrangement of protein atoms in three-dimensional space forming a coactivator binding site

pocket or cavity. As described by Apriletti, et al., supra, residues forming the coactivator binding site on nuclear receptors are amino acids that correspond to (i.e., the same as or equivalent to) human TR residues of C-terminal helix 3 (Ile280, Thr281, Val283, Val284, Ala287, and Lys288), helix 4 (Phe293), helix 5 (Gln301, Ile302, Leu305, Lys306), helix 6 (Cys309), and helix 12 (Pro453, Leu454, Glu457, Val458 and Phe459), as shown in Figure 8. The coactivator binding site is highly conserved among the nuclear receptor super family. Thus, this site corresponds to a surprisingly small cluster of residues on the surface of the LBD that form a prominent hydrophobic cleft. The hydrophobic cleft is formed by hydrophobic residues corresponding to human TR residues of C-terminal helix 3 (Ile280, Val283, Val284, and Ala287), helix 4 (Phe293), helix 5 (Ile302 and Leu305), helix 6 (Cys309), and helix 12 (Leu454, Val458 and Phe459). This hydrophobic cleft of the coactivator binding site is also highly conserved among the nuclear receptor super family.

Based upon the Examples set forth herein, residues forming the coactivator binding site on the estrogen receptor were found to correspond to those positions described above for the human TR. Accordingly, the residues forming the coactivator binding site on ERα are the human ERα residues of C-terminal helix 3 (Leu354, Val355, Met357, Ile358, Ala361, and Lys362), helix 4 (Phe367), helix 5 (Gln375, Val376, Leu379, Glu380), helix 6 (Trp383), and helix 12 (Asp538, Leu539, Glu542, Met543 and Leu544), as shown in Figure 8. As noted above for the nuclear receptor family in general, this site corresponds to residues on the surface of the LBD that form a prominent hydrophobic cleft, formed by hydrophobic residues corresponding to human ERα residues of C-terminal helix 3 (Leu354, Met357, Ile358 and Ala361), helix 4 (Phe367), helix 5 (Val376, Leu379), helix 6 (Trp383), and helix 12 (Leu539, Met543 and Leu544). This corroborates the data presented by Apriletti, et al., supra, for the nuclear receptor family.

Structural analysis has revealed the mechanisms by which tamoxifen and other SERMs bind the ligand binding domain and block coactivator binding and hence transcriptional activity. By this, an understanding of ligand and coactivator binding has also been achieved. Therefore, the coactivator binding site residues described above are useful in designing coactivator mimics that have broad application in the methods of the instant invention. Such "coactivator mimics" are peptides or polypeptides that mimic the coactivator binding site recognition area on the surface of a coactivator such that a "coactivator mimic" acts as a competitive inhibitor of coactivator binding to the coactivator binding site. Coactivator mimics can be used in an assay

to determine receptor activity and hence the agonist or antagonist nature of a test compound, in that an agonist will permit a coactivator mimic to bind to the coactivator binding site, while an antagonist will prevent such binding. In addition, such coactivator mimics may have therapeutic utility when administered in combination with an agonist compound of the invention.

Another embodiment of the invention pertains to a method of identifying a compound that modulates ligand binding to a nuclear receptor, typically by binding to the ligand binding domain. This method comprises the steps of modeling test compounds that fit spatially into a nuclear receptor ligand binding domain of interest using an atomic structural model of the estrogen receptor α ligand binding domain or portion thereof, screening the test compounds in an assay characterized by binding of a test compound to the binding domain, and identifying a test compound that modulates ligand binding to said nuclear receptor, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human estrogen receptor α Met343, Leu346, Ala350, Glu353, Leu384, Leu387, Leu391, Arg394, Phe404, Met421, Leu428, Gly521, His524, Leu525 and Met528, preferably Met343, Met421, His524, Leu525 and Met528. In the preferred method, the nuclear receptor is ER, TR, GR or PR. The screening is typically *in vitro* such as by high throughput screening. Suitable test compounds can be designed or obtained from a library of compounds, and include, by means of illustration and not limitation, small organic molecules, peptides and peptidomimetics. The test compounds can be either agonists or antagonists of ligand binding.

The invention also includes compositions and methods for identifying key residues within the ligand binding domains of nuclear receptors. The methods involve examining the surface of a nuclear receptor of interest to identify residues that modulate ligand and/or coactivator binding. The residues can be identified by homology to the key residues on the LBD of human ERα described herein. A preferred method is alignment with the residues of any nuclear receptor corresponding to (i.e., equivalent to) human ERα residues of Met343, Leu346, Ala350, Glu353, Leu384, Leu387, Leu391, Arg394, Phe404, Met421, Leu428, Gly521, His524, Leu525 and Met528, preferably Met343, Met421, His524, Leu525 and Met528. Overlays and superpositioning with a three-dimensional model of a nuclear receptor LBD, or a portion thereof that contains these or corresponding residues, also can be used for this purpose. For example, three-dimensional structures of TR, GR and PR LBDs can be used for this purpose. For example, nuclear receptors identifiable by homology alignment include normal nuclear receptors or proteins structurally related to nuclear receptors found in humans, natural mutants of nuclear

receptors found in humans, normal or mutant receptors found in animals, as well as non-mammalian organisms such as pests or infectious organisms, or viruses.

Alignment and/or modeling also can be used as a guide for the placement of mutations on the LBD surface to characterize the nature of the site in the context of a cell. Selected residues are mutated to preserve global receptor structure and solubility in the case of an agonist, or to disassemble such structure and permit helix 12 to unwind, as is the case with an antagonist. Mutants can be tested for ligand binding as well as the relative change in strength of the binding interaction. Ligand-dependent coactivator interaction assays also can be tested for this purpose, such as those described herein.

In particular, the present invention relates to the structural and functional effects on the estrogen receptor's LBD, of the binding of two chemically-related compounds, the agonist, diethylstilbestrol (DES), and the selective antagonist 4-hydroxytamoxifen (OHT), the active metabolite of tamoxifen. As described in the Examples, mutagenesis and binding studies, coupled with analysis of atomic models derived from cocrystals, reveals the structure of the human estrogen receptor α ligand binding domain (ERα LBD) co-crystallized with a peptide molecule comprising a GRIP1 NR Box II peptide sequence (SEQ ID NO:4) (i.e., a peptide derived from the NR Box II region of the p160 coactivator GRIP1) bound to the coactivator binding site and the agonist, DES. Also revealed is the structure of the ERα LBD co-crystallized with the antagonist, OHT. The Examples provide the 2.03Å resolution crystal structure of the hERα LBD bound to DES and the coactivator and the 1.9Å x-ray crystal structure of the hERα LBD bound to OHT, i.e., the crystals defract with at least 2.03Å or 1.9Å resolution, respectively.

In yet another aspect of the invention, compounds of interest are discovered, i.e., agonists or antagonists of ligand binding are identified, by a method for identifying an agonist or antagonist of ligand binding to a nuclear receptor. The method comprises the steps of providing the atomic coordinates of the ERα LBD or portion thereof to a computerized modeling system, modeling compounds which fit spatially into the LBD, and identifying in an assay for nuclear receptor activity a compound which increases or decreases the activity of the nuclear receptor by binding the LBD of the nuclear receptor. Preferably, the atomic coordinates are of the amino acid residues corresponding to residues of human estrogen receptor α Met343, Leu346, Ala350, Glu353, Leu384, Leu387, Leu391, Arg394, Phe404, Met421, Leu428, Gly521, His524, Leu525 and Met528, preferably Met343, Met421, His524, Leu525 and Met528.

Compounds of particular interest fit spatially and preferentially into the ligand binding domain. By "its spatially and preferentially" is intended that a compound possesses a three-dimensional structure and conformation for selectively interacting with a nuclear receptor LBD. Compounds that fit spatially and preferentially into the LBD interact with amino acid residues forming the hydrophobic cleft of this site. The present invention also includes a method for identifying a compound capable of selectively modulating nuclear receptor activity. The method comprises the steps of modeling test compounds that fit spatially and preferentially into the LBD of a nuclear receptor of interest using an atomic structural model of a nuclear receptor, screening the test compounds in an assay for nuclear receptor activity characterized by preferential binding of a test compound to the LBD of a nuclear receptor, and identifying a test compound that selectively modulates the activity of a nuclear receptor. Such receptor-specific compounds are selected that exploit differences between the LBDs of one type of nuclear receptor versus a second type of nuclear receptor.

The invention also is applicable to generating new compounds that distinguish nuclear receptor isoforms. This can facilitate generation of either tissue-specific or function-specific compounds. For instance, GR subfamily members have usually one receptor encoded by a single gene, although there are exceptions. For example, there are two PR isoforms, A and B, translated from the same mRNA by alternate initiation from different AUG codons. There are two GR forms, one of which does not bind ligand. This method is especially applicable to the ER subfamily which usually has several receptors that are encoded by at least two (ER: α, β) genes or have alternate RNA splicing.

The receptor-specific compounds of the invention preferably interact with conformationally constrained residues of the LBD that are conserved among one type of nuclear receptor compared to a second type of nuclear receptor. "Conformationally constrained" is intended to refer to the three-dimensional structure of a chemical or moiety thereof having certain rotations about its bonds fixed by various local geometric and physical-chemical constraints. Conformationally constrained structural features of a LBD include residues that have their natural flexible conformations fixed by various geometric and physical-chemical constraints, such as local backbone, local side chain, and topological constraints. These types of constraints are exploited to restrict positioning of atoms involved in receptor-coactivator recognition and binding.

The present invention also provides for a computational method using three dimensional models of nuclear receptors based on crystals of nuclear receptors. Generally, the computational method of designing a nuclear receptor ligand determines which amino acid or amino acids of a nuclear receptor LBD interact with a chemical moiety (at least one) of the ligand using a three dimensional model of a crystallized protein comprising a nuclear receptor LBD with a bound ligand, and selecting a chemical modification (at least one) of the chemical moiety to produce a second chemical moiety with a structure that either decreases or increases an interaction between the interacting amino acid and the second chemical moiety compared to the interaction between the interacting amino acid and the chemical moiety. In the instant invention, crystal structures of the hERα with DES/peptide and with OHT, have shown that amino acid residues that correspond to hERα Met343, Leu346, Ala350, Glu353, Leu384, Leu387, Leu391, Arg394, Phe404, Met421, Leu428, Gly521, His524, Leu525 and Met528, preferably Met343, Met421, His524, Leu525 and/or Met528, interact with at least one chemical moiety on the ligand.

Accordingly, one embodiment of the invention is a computational method of designing a nuclear receptor ligand where at least one amino acid residue of a nuclear receptor LBD that corresponds to human estrogen receptor α Met343, Leu346, Ala350, Glu353, Leu384, Leu387, Leu391, Arg394, Phe404, Met421, Leu428, Gly521, His524, Leu525 and Met528, preferably Met343, Met421, His524, Leu525 and Met528, interacts with at least one first chemical moiety of the ligand, comprising the step of selecting at least one chemical modification of the first chemical moiety to produce a second chemical moiety with a structure to either decrease or increase an interaction between the interacting amino acid and the second chemical moiety as compared to the interaction between the interacting amino acid and the first chemical moiety.

This computational method may further comprise determining a change in interaction between the interacting amino acid and the ligand after chemical modification of the first chemical moiety. The chemical modification can either enhance or reduce hydrogen bonding interaction, charge interaction, hydrophobic interaction, Van Der Waals interaction or dipole interaction between the second chemical moiety and the interacting amino acid as compared to the interaction between the first chemical moiety and the interacting amino acid.

Chemical modifications will often enhance or reduce interactions an atom of a LBD amino acid and an atom of an LBD ligand. Steric hindrance will be a common means of changing the interaction of the LBD binding cavity with the activation domain. Chemical modifications are preferably introduced at C-H, C- and C-OH position in ligands, where the

carbon is part of the ligand structure which remains the same after modification is complete. In the case of C-H, C could have 1, 2 or 3 hydrogens, but usually only one hydrogen will be replace. The H or OH are removed after modification is complete and replaced with the desired chemical moiety.

Such chemical modifications would preferably involve the addition of substituents, onto any of the free carbons of the A' ring of DES positioning these substituents to collide or bind preferentially with one or more residues that correspond to hERα Met343, Leu346, Ala350, Glu353, Leu384, Leu387, Leu391, Arg394, Phe404, Met421, Leu428, Gly521, His524, Leu525 and Met528, preferably Met343, Met421, His524, Leu525 or Met528. Typical substituents are hydrophobic groups, including by way of example and not limitation, alkyl groups such as ethyl, propyl, isopropyl, etc., and aromatic groups such as benzyl, etc.

In practice, one would start with a known ligand for the nuclear receptor of interest as the chemical backbone, upon which to base agonist/antagonist design. The known ligand would be modified as described above. For example 17β-estradiol is an endogenous ligand for the hERα. In the case of estradiol, positions of interest are C6α, C7α, C12α, C15α, C16α and C17α. Modifications at one or more of these free carbons on 17β-estradiol's backbone would affect the ligand's interactions with one or more of the Met343, Leu346, Ala350, Glu353, Leu384, Leu387, Leu391, Arg394, Phe404, Met421, Leu428, Gly521, His524, Leu525 and Met528, preferably Met343, Met421, His524, Leu525 and Met528 residues, either providing for enhancing interaction, which would be the basis for agonist design, or reduced interaction, which would be the basis for antagonist design.

Other chemical backbones of other known ligands could be used in a similar manner. For example, other known agonists include diethylstilbestrol (synthetic), moxestrol (synthetic), mesohexestrol (synthetic), coumestrol (clover), Δ^9-THC (cannabis), o,p-DDT (insecticide), zearalenone (fungal) and kepone (insecticide). Known estrogen receptor antagonists include the ICI series of modified steroids such as ICI 164,384 and EM800. Known SERM's include tamoxifen, raloxifene and GW5638.

Alternatively known agonists could be positioned in the ligand binding pocket through computational or manual docking. Positions for substitution would then be selected based on the predicted binding orientation of these compounds. In addition, hybrid molecules could be generated that also possessed side chains that prevented helix 12 from adopting the agonist-

bound position. Novel SERMs can be produced by varying the strength of two different effects: the helix 12 displacement and the secondary structure disorganization.

Previous efforts to make antagonists have involved attachment of large bulky substituents to agonists, typically through trial and error, and the drug design methods described herein provide an alternative strategy of ligand design that may be critical for developing new potential antagonists.

For modeling, docking algorithms and computer programs that employ them can be used to identify compounds that fit into the ligand binding domain. For example, docking programs can be used to predict how a molecule of interest can interact with the nuclear receptor LBD. Fragment-based docking also can be used in building molecules de novo inside the LBD, by placing chemical fragments that complement the site to optimize intermolecular interactions. The techniques can be used to optimize the geometry of the binding interactions. This design approach has been made possible by identification of the LBD structure thus, the principles of molecular recognition can now be used to design a compound which is complementary to the structure of this site. Compounds fitting the LBD serve as a starting point for an iterative design, synthesis and test cycle in which new compounds are selected and optimized for desired properties including affinity, efficacy, and selectivity. For example, the compounds can be subjected to addition modification, such as replacement and/or addition of R-group substituents of a core structure identified for a particular class of binding compounds, modeling and/or activity screening if desired, and then subjected to additional rounds of testing.

Computationally small molecule databases can be screened for chemical entities or compounds that can bind in whole, or in part, to a nuclear receptor ligand binding domain of interest. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity (DesJalais, et al., J. Med. Chem. 31:722-729 (1988)) or by estimated interaction energy (Meng, et al., J. Comp. Chem. 13:505-524 (1992)). The molecule databases include any virtual or physical database, such as electronic and physical compound library databases, and are preferably used in developing compounds that modulate coactivator binding.

Compounds can be designed intelligently by exploiting available structural and functional information by gaining an understanding of the quantitative structure-activity relationship (QSAR), using that understanding to design new compound libraries, particularly focused libraries having chemical diversity of one or more particular groups of a core structure.

and incorporating any structural data into that iterative design process. For example, one skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with the ligand binding domain of a nuclear receptor of interest. This process may begin by visual inspection of, for example, the LBD on the computer screen. Selected fragments or chemical entities may then be positioned into all or part of the site. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force-fields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting chemical entity fragments or whole compounds. These include: GRID (Goodford, J. Med. Chem. 28:849-857 (1985), available from Oxford University, Oxford, UK); MCSS (Miranker, et al., "Proteins: Structure, Function and Genetics" 11:29-34 (1991), available from Molecular Simulations, Burlington, MA); AUTODOCK (Goodsell, et al., "Proteins: Structure, Function and Genetics" 8:195-202 (1990), available from Scripps Research Institute, La Jolla, CA); and DOCK (Kuntz, et al, J. Mol. Biol. 161:269-288 (1982), available from University of California, San Francisco, CA).

Additional commercially available computer databases for small molecular compounds include Cambridge Structural Database and Fine Chemical Database (Rusinko, Chem. Des. Auto. News 8:44-47 (1993)).

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound. Assembly may be proceeded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of a nuclear receptor. This can be followed by manual model building using software such as Quanta or Sybyl.

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include: CAVEAT (Bartlett, et al., "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules", in Molecular Recognition in Chemical and Biological Problems, Special Pub., Royal Chem. Soc. 78:182-196 (1989), available from the University of California, Berkeley, CA); 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, CA, reviewed in Martin, J. Med. Chem. 35:2145-2154 (1992)); and HOOK (available from Molecular Simulations, Burlington, MA).

In addition to building a compound in a step-wise fashion, one fragment or chemical entity at a time as described above, compounds that bind to a ligand binding domain of interest also may be designed as a whole or de novo using either an empty LBD or optionally including some portion(s) of a molecule known to bind to the site, such as a known ligand. These methods include: LUDI (Bohm, J. Comp. Aid. Molec. Design 6:61-78 (1992), available from Biosm Technologies, San Diego, CA); LEGEND (Nishibata, et al., Tetrahedron 47:8985 (1991), available from Molecular Simulations, Burlington, MA); and LeapFrog (available from Tripos Associates, St. Louis, MO).

Other molecular modeling techniques may also be employed in accordance with this invention. See, for example, Cohen, et al., J. Med. Chem. 33:883-894 (1990) and Navia, et al., Current Opinions in Structural Biology 2:202-210 (1992). For example, where the structures of test compounds are known, a model of the test compound may be superimposed over the model of the structure of the invention. Numerous methods and techniques are known in the art for performing this step, any of which may be used. See, for example, Farmer, "Drug Design" 10:119-143, Ariens, ed., Academic Press, New York (1980); U.S. Patent No. 5,331,573; U.S. Patent No. 5,500,807; Verlinde, Structure 2:577-587 (1994); and Kuntz, et al., Science 257:1078-1082 (1992). The model building techniques and computer evaluation systems described herein are not a limitation on the present invention.

Using these computer modeling systems a large number of compounds may be quickly and easily examined and expensive and lengthy biochemical testing avoided. Moreover, the need for actual synthesis of many compounds can be substantially reduced and/or effectively eliminated.

Compounds identified through modeling can be screened in assays such as are well known in the art. Such assays, which include biological assays, are characterized by binding of the compound to a ligand binding domain of interest for ligand binding activity. Screening can be, for example, *in vitro*, in cell culture, and/or *in vivo*. Biological screening preferably centers on activity-based response models, binding assays (which measure how well a compound binds to the receptor), and bacterial, yeast and animal cell lines (which measure the biological effect of a compound in a cell). The assays can be automated for high capacity-high throughput screening (HTS) in which large numbers of compounds can be tested to identify compounds with the desired activity.

As an example, *in vitro* binding assays can be performed in which compounds are tested for their ability to block the binding of a ligand, fragment, fusion or peptide thereof, to a ligand binding domain of interest. For cell and tissue culture assays, they may be performed to assess a compound's ability to block function of cellular coactivators, such as members of the p160 family of coactivator proteins, such as SRC-1, AIB1, RAC3, p/CIP, and GRIP1 and its homologues TIF 2 and NcoA-2, and those that exhibit receptor and/or isoform-specific binding affinity. In a preferred embodiment, compounds of the invention bind to a ligand binding domain with greater affinity than the endogenous ligands. Tissue profiling and appropriate animal models also can be used to select compounds. Different cell types and tissues also can be used for these biological screening assays. Suitable assays for such screening are described herein and in Shibata, et al., Recent Prog. Horm. Res. 52:141-164 (1997); Tagami, et al., Mol. Cell. Biol. 17(5):2642-2648 (1997); Zhu, et al., J. Biol. Chem. 272(14):9048-9054 (1997); Lin, et al., Mol. Cell. Biol. 17(10):6131-6138 (1997); Kakizawa, et al., J. Biol. Chem. 272(38):23799-23804 (1997); and Chang, et al., Proc. Natl. Acad. Sci. USA 94(17):9040-9045 (1997), which references are incorporated herein in their entirety by reference.

The compounds selected can have agonist and/or antagonistic properties. The compounds also include those that exhibit new properties with varying mixtures of agonist and antagonist activities, depending on the effects of altering ligand binding in the context of different activities of nuclear receptors, either hormone-dependent or hormone-independent, which are mediated by proteins other than coactivators, and which interact with the receptors at locations other than the coactivator binding site. The compounds also include those, which through their binding to receptor locations that are conformationally sensitive to hormone binding, have allosteric effects on the receptor by stabilizing or destabilizing the hormone-bound conformation of the receptor, or by directly inducing the same, similar, or different conformational changes induced in the receptor by the binding of hormone.

Of particular interest is use of such compounds in a method of modulating nuclear receptor activity in a mammal by administering to a mammal in need thereof a sufficient amount of a compound that fits spatially and preferentially into a ligand binding domain of a nuclear receptor of interest. By "modulating" is intended increasing or decreasing activity of a nuclear receptor. For example, pre-clinical candidate compounds can be tested in appropriate animal models in order to measure efficacy, absorption, pharmacokinetics and toxicity following standard techniques known in the art. Compounds exhibiting desired properties are then tested

in clinical trials for use in treatment of various nuclear receptor-based disorders. These include ER-based disorders, such as postmenopausal symptoms and cancer resulting from loss of estrogen production, and osteoporosis and cardiovascular disease stemming from traditional estrogen replacement therapy. Others include GR-based disorders including Type II diabetes and inflammatory conditions such as rheumatic diseases.

Although for many nuclear receptors, the goal is to discover novel synthetic agonists or antagonists, it is important to realize the value for some nuclear receptors, especially the estrogen receptor, of developing compounds that have the desired agonist and antagonist effects in target tissues. Such compounds can be discovered and/or designed by the methods described herein, then screened for tissue specificity by methods that are well known in the art. For example, there is a great need for the improvement of existing therapies and the development of new agonists that act like estrogen in cardiovascular and brain tissue and bone, and new antagonists that act upon the estrogen receptor in uterine and breast tissue. Ideally, a compound will have more than one of these traits, i.e., a compound will act as an agonist in one tissue, while acting as an antagonist in another tissue. While the tissue-selective antagonism of SERMs such as OHT and RAL is the result of numerous factors (Grainger, et al., Nature Medicine 2(4):381-385 (1996); Grese, et al., supra; and Jordan, J. Natl. Cancer Inst. 90:967-71 (1998)), dissection of the mechanisms of action of these ligands requires a comprehensive understanding of how they act on the LBD and regulate its interactions with other cellular factors. The instant invention shows, unexpectedly, that ligand-mediated structural perturbations in and around the ligand binding pocket, and not simply side chain effects, contribute to receptor antagonism. Accordingly, by adjusting the balance between these two effects provides a novel strategy for the design of improved SERMs.

With this knowledge, it is of particular interest to design therapeutic compounds that will distort at least one amino acid residue corresponding to residues of human estrogen receptor α Met343, Leu346, Ala350, Glu353, Leu384, Leu387, Leu391, Arg394, Phe404, Met421, Leu428, Gly521, His524, Leu525 and Met528, preferably Met343, Met421, His524, Leu525 and Met528. Accordingly, one aspect of the invention is a method of modulating nuclear receptor activity in a mammal by administering to a mammal in need thereof a sufficient amount of a ligand that fits spatially and preferentially into a ligand binding domain of a nuclear receptor of interest, wherein the ligand is designed by a computational method where at least one amino acid residue of a nuclear receptor LBD that corresponds to hERα Met343, Leu346, Ala350, Glu353, Leu384,

Leu387, Leu391, Arg394, Phe404, Met421, Leu428, Gly521, His524, Leu525 and Met528, preferably Met343, Met421, His524, Leu525 and Met528, interacts with at least one first chemical moiety of the ligand. Such a method involves selecting at least one chemical modification of the first chemical moiety to produce a second chemical moiety with a structure that either decreases or increases an interaction between the interacting amino acid and the second chemical moiety as compared to the interaction between the interacting amino acid and the first chemical moiety.

Compounds designed by this method can be either agonists or antagonists and the method of modulating nuclear receptor activity can comprise administering an antagonist alone, an agonist alone or an agonist in combination with a coactivator or a compound that mimics a coactivator by binding to the coactivator binding site.

The coactivator can be a known coactivator. The coactivator mimic can be designed by a computational method where at least one amino acid residue of a nuclear receptor coactivator binding site that corresponds to hERα helix 3 residues Leu354, Val355, Met357, Ile358, Ala361 and Lys362, helix 4 residue Phe367, helix 5 residues Gln375, Val376, Leu379 and Glu380, helix 6 residue Trp383, and helix 12 residues Asp538, Leu539, Glu542, Met543 and Leu544, interacts with at least one first chemical moiety of the coactivator mimic. The method involves selecting at least one chemical modification of the first chemical moiety to produce a second chemical moiety with a structure that either decreases or increases an interaction between the interacting amino acid and the second chemical moiety as compared to the interaction between the interacting amino acid and the first chemical moiety.

Use of an agonist in combination with a coactivator or coactivator mimic also provides a unique strategy for delivering therapeutics that have novel tissue-specific effects. For example, coactivator mimics can be designed to bind into the site involved in transcriptional activity only when helix-12 is in its agonist bound state. If such coactivator mimics are specific for this site of a particular receptor, it is possible to selectively inhibit that receptor only in the presence of agonist. This could lead to novel, tissue specific antagonism based on the levels of endogenous agonists. Agonists designed by the methods of the instant invention could be used in assay to determine the specificity of coactivator mimics. Alternatively, the effective levels in a given tissue could be modulated by giving known antagonists or antagonists designed by the methods of the instant invention. The crystal structure of the LBD/DES/GRIP1 peptide complex, described herein, precisely defines the binding site that would need to be targeted.

As noted above and as exemplified in the Examples, ER LBDs are co-crystallized with a peptide molecule comprising a coactivator GRIP1 NR Box II peptide sequence (SEQ ID NO:4) bound to the coactivator binding site and DES with the cocrystal structure refined to a resolution of 2.03Å and co-crystallized with OHT with the cocrystal structure refined to a resolution of 1.9Å. Accordingly, the invention also provides for cocrystals made from nuclear receptor ligand binding domains with a ligand bound to the ligand binding domain and a molecule bound to the coactivator binding site. Preferably the cocrystal structure is refined to a resolution greater than 3.6Å, i.e., having a resolution value less than 3.6Å. More preferably the cocrystal structure is refined to greater than 3.4Å, 3.2Å, 3.0Å, 2.8Å, 2.6Å, 2.4Å, 2.2Å, even more preferably to a resolution greater than 2.03Å. The invention further provides for cocrystals made from nuclear receptor ligand binding domains with a ligand bound to the ligand binding domain. Preferably the cocrystal structure is refined to a resolution greater than 3.6Å, i.e., having a resolution value less than 3.6Å. More preferably the cocrystal structure is refined to greater than 3.4Å, 3.2Å, 3.0Å, 2.8Å, 2.6Å, 2.4Å, 2.2Å, 2.0Å, even more preferably to a resolution greater than 1.9Å.

Crystals are made from purified nuclear receptor LBDs that are usually expressed by a cell culture, such as E. coli. E. coli is often a preferred expression system. The thyroid receptor was successfully expressed in E. coli in Apriletti, et al., supra. However, it has long been believed that a human heat shock protein was required for successful recombinant expression of the estrogen receptor. Therefore, it was quite unexpected to find that the estrogen receptor could be expressed as an active protein in E. coli.

Preferably, different crystals (cocrystals) for the same nuclear receptor are separately made using different coactivators-type molecules, such as protein fragments, fusions or small peptides. The coactivator-type molecules preferably contain NR-box sequences necessary for binding to the coactivator binding site, or derivatives of NR-box sequences. Other molecules can be used in co-crystallization, such as small organics that bind to the coactivator or hormone binding site(s). Heavy atom substitutions can be included in the LBD and/or a co-crystallizing molecule.

After the three dimensional structure of the cocrystal is determined, the structural information can be used in computational methods to design synthetic compounds for the nuclear receptor, and further structure-activity relationships can be determined through routine testing using the assays described herein and known in the art.

Since nuclear receptor LBDs may crystallize in more than one crystal form the structure coordinates of such receptors or portions thereof, as provided in Appendices 1 and 2, are particularly useful to solve the structure of those other crystal forms of nuclear receptors. They may also be used to solve the structure of mutants or co-complexes of nuclear receptors having sufficient homology.

One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure, may be determined using the structure coordinates of this invention as provided in Appendices 1 and 2. The Appendix 1 coordinates for the DES-ERα LBD-GRIP1 NR Box II peptide complex and for the Appendix 2 coordinates for the OHT-ERα LBD complex have been deposited with the Brookhaven National Laboratory Protein Data Bank, and have been assigned Brookhaven Protein Data Bank Accession Numbers 2erd and 2ert, respectively. This method will provide an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information *ab initio*.

Atomic coordinate information gleaned from the crystals of the invention can be stored. In a preferred embodiment, the information is provided in the form of a machine-readable data storage medium. This medium contains information for constructing and/or manipulating an atomic model of a ligand binding domain or portion thereof. For example, the machine readable data for the ligand binding domain comprises structure coordinates of amino acids corresponding to hERα Met343, Leu346, Ala350, Glu353, Leu384, Leu387, Leu391, Arg394, Phe404, Met421, Leu428, Gly521, His524, Leu525 and Met528, preferably Met343, Met421, His524, Leu525 and Met528, or a homologue of the molecule or molecular complex comprising the site. The homologues comprise a LBD that has a root mean square deviation from the backbone atoms of the amino acids of not more than 1.5Å. A preferred molecule or complex represents a compound bound to the LBD.

The machine-readable data storage medium can be used for interactive drug design and molecular replacement studies. For example, a data storage material is encoded with a first set of machine-readable data that can be combined with a second set of machine-readable data. For molecular replacement, the first set of data can comprise a Fourier transform of at least a portion of the structural coordinates of the nuclear receptor or portion thereof of interest, and the second data set comprises an X-ray diffraction pattern of the molecule or molecular complex of interest. Using a machine programmed with instructions for using the first and second data sets a portion or all of the structure coordinates corresponding to the second data can be determined.

Protein for crystals and assays described herein can be produced using expression and purification techniques described herein and known in the art. For example, high level expression of nuclear receptor LBDs can be obtained in suitable expression hosts such as E. coli. Expression of LBDs in E. coli, for example, includes the ERα LBD and other nuclear receptors, including GR and PR. Yeast and other eukaryotic expression systems can be used with nuclear receptors that bind heat shock proteins as these nuclear receptors are generally more difficult to express in bacteria, with the exception of ER, which can be expressed in bacteria. Representative nuclear receptors or their ligand binding domains have been cloned and sequenced: human ER (as described in Seielstad, et al., Molecular Endocrinology 9(6):647-658 (1995), incorporated herein by reference), human GR, and human PR. The LBD for each of these receptors has been identified.

Coactivator proteins can be expressed using techniques known in the art, particularly members of the p160 family of coactivator proteins that have been cloned and/or expressed previously, such as SRC-1, AIB1, RAC3, p/CIP, and GRIP1 and its homologues TIF 2 and NcoA-2. A preferred method for expression of coactivator protein is to express a fragment that retains transcriptional activation activity using the "Song and Fields" method (also referred to as the "yeast 2-hybrid" method) as described in publications by Hong, et al., Mol. Cell. Biol. 17:2735-44 (1997) and Proc. Natl. Acad. Sci. USA 93(10):4948-52 (1996)), for GRIP1 expression, which references are incorporated herein by reference.

The proteins can be expressed alone, as fragments of the mature or full-length sequence, or as fusions to heterologous sequences. For example, ERα can be expressed without any portion of the DBD or amino-terminal domain. Portions of the DBD or amino-terminus can be included if further structural information with amino acids adjacent the LBD is desired. Generally, for the ERα the LBD used for crystals will be less than 320 amino acids in length. Preferably, the ERα LBD will be at least 220 amino acids in length and most preferably at least 250 amino acids in length. For example the LBD used for crystallization can comprise amino acids spanning from 297 to 554 of the ERα.

Typically the LBDs are purified to homogeneity for crystallization. Purity of LBDs can be measured with sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE), mass spectrometry (MS) and hydrophobic high performance liquid chromatography (HPLC). The purified LBD for crystallization should be at least 97.5 % pure, preferably at least 99.0% pure, and more preferably at least 99.5% pure.

Initially, purification of the unliganded receptor can be obtained by conventional techniques, such as hydrophobic interaction chromatography (HPLC), ion exchange chromatography (HPLC), and heparin affinity chromatography. To achieve higher purification for improved crystals of nuclear receptors, especially the estrogen receptor, the receptors can be ligand-shift-purified using a column that separates the receptor according to charge, such as an ion exchange or hydrophobic interaction column, and then bind the eluted receptor with a ligand, especially an agonist. The ligand induces a change in the receptor's surface charge such that the liganded receptor elutes at a different position than the unliganded receptor. Usually saturating concentrations of ligand are used in the column and the protein can be preincubated with the ligand prior to passing it over the column. The structural studies detailed herein indicate the general applicability of this technique for obtaining super-pure nuclear receptor LBDs for crystallization.

Purification can also be accomplished by use of a purification handle or "tag," such as with a histidine amino acid engineered to reside on the end of the protein, such as on the N-terminus, and then using a nickel or cobalt chelation column for purification. (Janknecht, Proc. Natl. Acad. Sci. USA, 88:8972-8976 (1991)) incorporated by reference. Typically purified LBD, such as ERα LBD, is equilibrated at a saturating concentration of ligand at a temperature that preserves the integrity of the protein. Ligand equilibration can be established between 2 and 37°C, although the receptor tends to be more stable in the 2-20°C range. Preferably crystals are made with the hanging drop methods detailed herein. Regulated temperature control is desirable to improve crystal stability and quality. Temperatures between 4 and 25°C are generally used and it is often preferable to test crystallization over a range of temperatures. The crystals are then subjected to vapor diffusion and bombarded with x-rays to obtain x-ray diffraction pattern following standard procedures.

For co-crystallization with a ligand that binds the ligand binding domain, alone or in conjunction with a peptide that binds to the coactivator binding site, various concentrations of ligands and peptides containing a sequence that binds to a coactivator binding site of a nuclear receptor of interest can be used in microcrystallization trials, and the appropriate compounds selected for further crystallization. Ligands and peptides can be assayed for binding to the ligand binding domain and coactivator binding sites of a nuclear receptor of interest by any number of techniques, including those assays described herein. For crystallization trials with the ERα LBD, the hanging drop vapor diffusion method is preferred. Conditions of pH, solvent and

solute components and concentrations and temperature can be adjusted, for instance, as described in the Examples. In the handing drop method, to obtain suitable crystals for x-ray diffraction analysis, seeding of prepared drops with microcrystals of the complex can be used. Collection of structural information can be determined by molecular replacement using the structure of the ERα LBD determined herein. The structure is refined following standard techniques known in the art.

There are many uses and advantages provided by the present invention. For example, the methods and compositions described herein are useful for identifying peptides, peptidomimetics or small natural or synthetic organic molecules that modulate nuclear receptor activity. The compounds are useful in treating nuclear receptor-based disorders. Methods and compositions of the invention also find use in characterizing structure/function relationships of natural and synthetic ligands.

The following discussion of provides an understanding of the basis for the examples, along with the results obtained and/or the conclusions reached.

As described above, many coactivators recognize agonist bound nuclear receptor LBDs through the sequence LXXLL (SEQ ID NO:1), where L is leucine and X is any amino acid (the NR box). The structure of the DES-hERα LBD-GRIP1 peptide complex reveals that the LXXLL motif (SEQ ID NO:1) forms the core of a short amphipathic α helix which is recognized by a highly complementary hydrophobic groove on the surface of the receptor. In agreement with the conclusions of other mutational and structural studies (Brzozowski, et al., supra and Feng, et al., supra), it is believed that this peptide binding groove formed by residues from helices 3, 4, 5 and 12 and the turn between helices 3 and 4 is the surface of ERα involved with transcriptional activity, i.e., the coactivator binding site. Further, structural studies of the complex between TRβ and the GRIP1 NR box II peptide and biochemical studies of GRIP1 binding to TRβ and GR (Darimont, et al., supra) and study of the general features of the PPARγ/SRC-1 peptide complex (Nolte, et al., supra) are similar to those of the ERα/GRIP1 NR box II peptide complex described herein, suggesting that the mechanisms of NR box recognition are conserved across the nuclear receptor family.

Of the eleven AF-2 residues whose side chains interact with the coactivator helix (Figure 3A), only four (Lys 362, Leu 379, Gln 375 and Glu 542) are highly conserved across the nuclear receptor family (Wurtz, et al., supra). The side chains of Gln 375 and Leu 379 are predominantly buried even in the absence of GRIP1 binding and appear to form integral parts of

the architecture of the surface involved in transcriptional activity. In contrast, the side chains of Lys 362 and Glu 542 are largely solvent exposed in the absence of coactivator and make both nonpolar contacts and the only receptor-mediated polar interactions with the coactivator helix. These two capping interaction residues are perfectly positioned at opposite ends of the coactivator binding site groove not only to stabilize the main chain conformation of the coactivator but also to function as a molecular caliper; the 15Å distance between Lys 362 and Glu 542 is well suited to measure off the ~11Å axial length of the short, two-turn coactivator α helix (Figure 3C). Similar receptor-mediated capping interactions have also been observed in a complex between the TRβ LBD and the NR box II peptide (Darimont, et al., supra). Mutation of either of these two residues severely cripples coactivator binding by ERα as well as by TRβ (see the Examples, Apriletti, et al., supra and Feng, et al., supra and Henttu, et al., supra). Hence, the formation of helix capping interactions may be a general feature of coactivator recognition by nuclear receptors.

The side chains of six hydrophobic AF-2 residues (Ile 358, Leu 372, Val 376, Leu 379, Leu 539 and Met 543) form a large part of the highly cooperative network of van der Waals contacts made by the receptor with the hydrophobic face of the coactivator helix (Figures 3A and 3C). Mutations in Ile 358, Val 376 and Leu 539 abrogate GRIP1 binding (see the Examples and Feng, et al., supra). Although these residues are, in general, more poorly conserved across nuclear receptors than either Lys 362 or Glu 542, their hydrophobic character, with the exception of Leu 372, is conserved. Since the different NR LBDs adopt the same overall fold (Moras, et al., Curr. Opin. Cell Biol. 10:384-91 (1998)), it follows that the hydrophobic regions of different nuclear receptor coactivator binding site surfaces are distinctly textured. In support of this hypothesis, the NR box II peptide used in crystallization inhibited binding of GRIP1 to the LBDs of the ERα, the TRβ and the glucocorticoid receptor (GR) with very different efficiencies (Ding, et al., supra).

The hydrophobic face of the NR box helix is formed by the side chains of the three motif leucines and the isoleucine preceding the motif (Ile 689). The functional importance of the conserved leucines in receptor binding has been demonstrated by numerous *in vitro* and *in vivo* studies. In contrast, the role of the residue preceding the motif in receptor binding has been poorly characterized. Both biochemical and structural data implicate Ile 689 as a key receptor binding determinant. In the crystal, only the side chains of the motif leucines and Ile 689 extensively contact the LBD in both noncrystallographic symmetry related peptides. Mutation of

Ile 689 to alanine reduces the ability of the peptide to inhibit the binding of GRIP1 to ERα by ~30 fold in a competition assay (data not shown). The side chain of Ile 689 lies in a rather chemically distinct environment; this residue forms van der Waals contacts with the aliphatic portion of the Asp 538 side chain, the side chain of Leu 539 and the γ-carboxylate of Glu 542 (Figures 1A and 3A). The proximity of this negatively charged moiety of Glu 542 to the hydrophobic side chain of Ile 689 should enhance the electrostatic potential of the side chain carboxylate and strengthen its stabilizing interactions with the N-terminus of the coactivator helix. Despite its apparently crucial role in receptor recognition, the identity of the residue immediately preceding known NR boxes is poorly conserved. This sequence variability should have effects not only on packing interactions with ERα but also on both the chemical environment and the critically important orientation of Glu 542. This should in turn translate into variations in affinity for the receptor. Indeed, the three NR boxes from GRIP1, which each contain a different residue preceding the LXXLL motif (SEQ ID NO:1), have differing affinities for ERα (Ding, et al., supra; Voegel, et al., EMBO J. 17:507-19 (1998)).

The NR boxes of TIF2, the human homologue of GRIP1, have been found to be partially functionally redundant despite their individual differences in receptor binding affinities. All three of NR boxes of TIF2 must be mutated to completely eliminate interaction with the ERα (Voegel, et al., EMBO J. 17:507-19 (1998)). Our data indicate that a single NR box peptide is sufficient to form a tight complex with a single ERα LBD. Yet p160 coactivators possess multiple NR boxes. A possible explanation for the presence of multiple NR boxes is that they provide coactivators with broad specificity. Receptor binding relies upon the intricate formation of multiple van der Waals interactions yet the various nuclear receptors appear to have different coactivator binding site surfaces. The different amino acids in the position immediately preceding the LXXLL motif (SEQ ID NO:1) might allow some degree of adaptability to these distinct surfaces; however, there may be no NR box sequence that is capable of efficiently binding to all nuclear receptors. Multiple NR boxes may therefore provide coactivators the diversity of interfaces necessary to recognize a variety of targets.

ERα transcriptional activity is blocked by antagonists such as OHT and RAL. The most striking feature of the structures of the OHT and RAL liganded ERα LBDs is that helix 12 is bound to the static region of the coactivator recognition groove (Figure 3B and (Brzozowski, et al., supra). A comparison of these two structures with the structure of the coactivator/LBD complex reveals that in the antagonist complexes, the region of helix 12 with an NR box-like

sequence (LXXML versus LXXLL) (SEQ ID NO:2 versus SEQ ID NO:1) functions as an intramolecular mimic of the coactivator helix (Figure 5 and Brzozowski, et al., supra). Consistent with the proposals of others (Brzozowski, et al., supra and Darimont, et al., supra), this disposition of helix 12 directly affects the structure and function of the surface responsible for transcriptional activity in two ways. First, because helix 12 residues form an integral part of the coactivator binding site surface, the surface is incomplete when helix 12 is in the antagonist-bound conformation. In particular, Leu 539, Glu 542 and Met 543 are incorrectly oriented for coactivator recognition. Second, residues from the static region of this surface are bound to helix 12 and are prevented from interacting with coactivator (Figures 3A and 3B).

The sequence similarity of helix 12 of the ERα LBD to the LXXLL motif (SEQ ID NO:1) appears to be unique among nuclear receptors. The identities of the residues in this region of helix 12 in other nuclear receptors, although generally hydrophobic in character, do not as closely resemble the sequence of an NR box as those of ERα (Wurtz, et al., supra). However, it is possible that an intramolecular inhibitor with a suboptimal recognition sequence would compete for coactivator binding given its extremely high local concentration.

The binding of OHT to the ERα promotes a helix 12 conformation that inhibits binding of the coactivator. OHT does not directly interact with any helix 12 residues (Figure 4B). Moreover, the structure of the LBD in the region of the coactivator binding site groove that interacts with helix 12 in the OHT complex is the same in the DES and E_2 complexes (Figures 3A, 3B and 5).

Numerous studies have demonstrated the importance of the OHT side chain in receptor antagonism (Jordan, et al., supra and Robertson, et al., J. Med. Chem. 25:167-71 (1982)). A comparison of the structures of the OHT and DES complexes reveals that the binding mode of the OHT side chain precludes the agonist-induced conformation of helix 12. The OHT side chain projects out of the ligand binding pocket between helices 3 and 11 (Figures 2B, 6B and 6C). As a result, the positioning of helix 12 over the ligand binding pocket, as it is in the agonist-bound conformation, would bury the positively charged dimethylamino group of the OHT side chain within a hydrophobic cavity and produce steric clashes between the dimethylaminoethyl region of side chain and the side chain of Leu 540.

In functional terms, OHT is not, however, simply "an agonist with a side chain". OHT binding promotes a conformation of the LBD that is distinct from that stabilized by either DES

or E_2 binding. These different conformations impose different restrictions on the positioning of helix 12.

Helices 3, 8 and 11 in the DES and E_2 complexes are between one to two turns longer than they are in the OHT complex (Figure 6A and (Brzozowski, et al., supra). Helix 11 ends at Cys 530 in the DES and E_2 complexes and it ends at Tyr 526 in the OHT complex. Helix 12 begins at Leu 536 in the OHT complex. This appears to be necessary; in the antagonist complex, Leu 536 forms a cooperative network of nonpolar contacts and hydrogen bonds with Glu 380 and Tyr 537 that stabilizes the N-terminus of helix 12 (Figure 1B). Therefore, if helix 12 were to bind the static region of the coactivator binding site in the presence of agonist, the loop connecting helices 11 and 12 would be required to span ~17Å over five residues. Although theoretically possible, this conformation would be highly strained and hence unlikely. In contrast, the longer loop connecting helices 11 and 12 in the OHT complex allows helix 12 to extend to the static region of the coactivator binding groove.

In the DES and E_2 complexes, helix 12 and the loop connecting helices 11 and 12 pack against helices 3 and 11, whereas they do not in the OHT complex (Figures 2A and 2B and (Brzozowski, et al., supra). A recently described structure of the E_2-LBD complex suggests that the longer helices in the DES and E_2 complexes are not dependent upon the interactions helix 12 forms in the agonist-bound conformation (Tanenbaum, et al., supra). In this structure, a crystal packing artifact forces helix 12 to contact a symmetry-related molecule. Helix 12 is clearly not positioned over the ligand binding pocket in this structure. Nevertheless, helices 3, 8 and 11 are longer than they are in the OHT complex (Figure 6A). Hence the longer helices of the agonist complexes occur independently of the positioning of helix 12 over the ligand binding pocket and are instead a direct result of agonist binding.

The secondary structure differences between the agonist complexes and the OHT complex arise from distinct arrangements of packing interactions induced by the different ligands. A cooperative network of van der Waals contacts, organized around DES or E_2, between various hydrophobic residues from helices 3, 7, 8 and 11 and the β hairpin appears to stabilize the longer helices in the agonist complexes (Figure 4A and 6D). The placement of the OHT B ring forces many of ligand binding pocket residues that surround it to adopt conformations that are dramatically different from those they adopt in either the DES or E_2 structures. As a result, many of the interresidue packing interactions present in the DES and E_2 structures are either absent or altered in the OHT structure (Figure 6D). These structural

distortions apparently force the main chain from residues 339 to 341, 421 to 423, and 527 to 530 (which form parts of helices 3, 8 and 11 respectively in the agonist structures) to adopt an extended conformation in the OHT structure (Figures 6A-D).

Therefore the binding of OHT has two distinct effects on the positioning of helix 12, each of which contributes to antagonism (Figure 7). Helix 12 is prevented from being positioned over the ligand binding pocket by the OHT side chain. In addition, the alternative packing arrangement of ligand binding pocket residues around OHT stabilizes a conformation of the LBD that permits helix 12 to reach the static region of the coactivator binding site and mimic bound coactivator.

These mechanisms do not appear to be specific to OHT. The side chain of RAL, like that of OHT, sterically hinders the agonist-bound conformation of helix 12 (Brzozowski, et al., supra). In addition, helix 11 appears to end at Met 528 in the RAL complex. This may result from the distortions in the binding pocket in the vicinity of His 524 directed by RAL binding (Brzozowski, et al., supra).

These results are supported by the experimental data provided in the examples below, which are also intended to illustrate various aspects of this invention. These examples do not limit the scope of this invention.

EXAMPLES

Example 1
Experimental Procedures

Protein Expression and Purification

The human ERα-LBD 297-554 was overexpressed as described previously (Seielstad, et al., Mol. Endocrinol. 9:647-658 (1995)) in BL21(DE3)pLysS cells transformed with a modified pET-23d-ERG vector that contained the sequence Met-Asp-Pro fused to residues 297 through 554 of the hERα (provided by Paul Sigler of Yale University). Clarified bacterial lysates were adjusted to 3 M in urea and 0.7 M in NaCl and then applied to a 10-ml column of estradiol-Sepharose (Greene, et al., Proc. Natl. Acad. Sci. USA 77:5115-5119 (1980); Landel, et al., Mol. Endocrinol. 8:1407-1419 (1994); Landel, et al., J. Steroid Biochem. Molec. Biol. 63:59-73 (1997)).

To carboxymethylate the solvent-accessible cysteines, the bound hERα-LBD was treated with 5 mM iodoacetic acid in 10 mM Tris, pH 8.1, 250 mM NaSCN (Hegy, et al., Steroids 61:367-373 (1996)). Protein was eluted with 3 x 10-5 M ligand (either DES or OHT) in 30-100

ml of 50 mM Tris, 1 mM EDTA, 1 mM DTT and 250 mM NaSCN, pH 8.5. The yield of hERα-LBD was typically close to 100% (Seielstad, et al., Biochemistry 34:12605-12615 (1995)). The affinity-purified material was concentrated and exchanged into 20 mM Tris, 1 mM EDTA, 4 mM DTT, pH 8.1 by ultrafiltration. The protein was bound to a Resource Q column (Pharmacia) and then eluted with a linear gradient of 25-350 mM NaCl in 20 mM Tris, pH 8.1, 1 mM DTT. The hERα-LBD-ligand complexes eluted at 150-200 mM NaCl. Pooled fractions were concentrated by ultrafiltration and analyzed by SDS-PAGE, native PAGE, and electrospray ionization mass spectrometry.

GST-pulldown Assays

A fusion between glutathione-S-transferase (GST) and amino acids 282-595 of hERα was constructed by subcloning the EcoRI fragment from pSG5 ERα-LBD (Lopez et al., submitted manuscript) into pGEX-3X (Pharmacia). The Ile 358-> Arg, Lys 362->Ala, and Leu 539->Arg mutations were introduced into the GST-LBD construct using the QuikChange Kit (Stratagene) according to the manufacturer's instructions. The Val 376->Arg and Glu 542->Lys mutations were created in the GST-LBD construct by subcloning the BsmI/HindIII fragments of derivatives of pSG5-ER-HEGO (Tora, et al., EMBO J. 8:1981-6 (1989)) into which these mutations had already been introduced. All constructs were verified by automated sequencing (University of Chicago Cancer Research Center DNA Sequencing Facility).

The wild-type and mutant GST-LBDs were expressed in BL21(DE3) cells. Total ligand binding activity was determined by a controlled pore glass bead assay (Greene, et al., Mol. Endocrinol. 2:714-726 (1988)) and protein levels were monitored by western blotting with a monoclonal antibody to hERα (H222). Cleared extracts containing the GST-LBDs were incubated in buffer alone (50 mM Tris, pH 7.4, 150 mM NaCl, 2 mM EDTA, 1 mM DTT, 0.5% NP-40 and a protease inhibitor cocktail) or with 1 μM of either DES or OHT for 1 hour at 4°C. Extract samples containing thirty pmol of GST-LBD were then incubated with 10 μl glutathione-Sepharose-4B beads (Pharmacia) for 1 hour at 4°C. Beads were washed five times with 20 mM HEPES, pH 7.4, 400 mM NaCl, and 0.05% NP-40. ^{35}S-labeled GRIP1 was synthesized by *in vitro* transcription and translation using the TNT Coupled Reticulocyte Lysate System (Promega) according to the manufacturer's instructions and pSG5-GRIP1 (provided by Michael Stallcup of the University of Southern California) as the template. Immobilized GST-LBDs were incubated for 2.5 hours with 2.5 μl aliquots of crude translation reaction mixture diluted in 300 μl of Tris-buffered saline (TBS). After five washes in TBS containing 0.05% NP-40, proteins were eluted

by boiling the beads for 10 minutes in sample buffer. Bound ^{35}S-GRIP1 was quantitated by fluorography following SDS-PAGE.

Crystallization and Data Collection

Crystals of the DES-hERα LBD-GRIP1 NR Box II peptide complex were obtained by hanging drop vapor diffusion. Prior to crystallization, the DES-hERα LBD (residues 297-554) complex was incubated with a 2-4 fold molar excess of the GRIP1 NR Box II peptide (SEQ ID NO:4) for 7-16 hr. Two μL samples of this solution were mixed with equal volume samples of reservoir buffer consisting of 25-27% (w/v) PEG 4000, 90 mM Tris (pH 8.75-9.0) and 180 mM Na Acetate and suspended over wells containing 800 μL of the reservoir buffer. After 4-7 days at 19-21°C, rod-like crystals were obtained. The coactivator complex crystals lie in the spacegroup $P2_1$ with cell dimensions a=54.09, b=82.22, c=58.04 and β=111.34. Two molecules each of the DES-LBD and the coactivator peptide form the asymmetric unit. A 200 μm x 40 μm x 40 μm crystal was transferred to a cryosolvent solution containing 25% (w/v) PEG 4000, 10% (w/v) ethylene glycol, 100 mM Tris (pH 8.5), 200 mM Na Acetate and 10 μM peptide and frozen in an N_2 stream at -170°C in a rayon loop. Diffraction data from this crystal were measured at -170°C using a 300 mm MAR image plate at the Stanford Synchrotron Radiation Laboratory (SSRL) at beamline 7-1 at a wavelength of 1.08Å.

Crystals of the hERα LBD complexed to OHT were obtained by the hanging drop vapor diffusion method. Equal volume aliquots (2 μL) of a solution containing 3.9 mg/mL protein-ligand complex and the reservoir solution containing 9% (w/v) PEG 8000, 6% (w/v) ethylene glycol, 50 mM HEPES (pH 6.7) and 200 mM NaCl were mixed and suspended over 800 μL of the reservoir solution. Hexagonal plate-like crystals formed after 4-7 days at 21-23°C. Both crystal size and quality were improved through microseeding techniques. These crystals belong to the space group $P6_522$ with cell parameters a=b=58.24Å and c=277.47Å. The asymmetric unit consists of a single LBD monomer; the dimer axis lies along a crystallographic two-fold. A single crystal (400 μm x 250 μm x 40 μm) was briefly incubated in a cryoprotectant solution consisting of 10% (w/v) PEG 8000, 25% (w/v) ethylene glycol, 50 mM HEPES (pH 7.0) and 200 mM NaCl and then flash frozen in liquid N_2 suspended in a rayon loop. Diffraction data were measured at -170°C using a 345 mm MAR image plate at SSRL at beamline 9-1 and at a wavelength of 0.98Å.

The images of both data sets were processed with DENZO and scaled with SCALEPACK (Otwinowski, et al., Methods Enzymol. 276:307-326 (1997)) using the default -3σ cutoff.

Structure Determination and Refinement

Initial efforts to determine the structure of the DES-LBD-GRIP1 NR Box II peptide complex utilized a low resolution (3.1Å) data set (data not shown). A self-rotation search implemented with POLARRFN ("The CCP4 suite: programs for protein crystallography", Acta Crystallogr. D 50:760-763 (1994)) indicated the presence of a noncrystallographic dyad. The two LBDs in the asymmetric were located by molecular replacement in AMoRe (CCP4, 1994) using a partial polyalanine model of the human RARγ LBD (Renaud, et al., supra) as the search probe (R=58.2%, CC=35.6% after placement of both monomers). Given that the model at this point was both inaccurate (r.m.s.d. 1.7Å between this model and the final model based on Cα positions) and incomplete (accounting for only ~45% of the total scattering matter in the asymmetric unit), an aggressive density modification protocol was undertaken. Iterative cycles of two-fold NCS averaging in DM (CCP4, 1994) interspersed with model building in MOLOC (Muller, et al., Bull. Soc. Chim. Belg. 97:655-667 (1988)) and model refinement in REFMAC (Murshudov, et al., Acta Crystallogr. D 53:240-255 (1997)) (using tight NCS restraints) were used to quickly build a model of the LBD alone. For this procedure, MAMA (Kleywegt, et al., "Halloween...masks and bones. In From First Map to Final Model", Bailey, et al, eds., Warrington, England, SERC Daresbury Laboratory, 1994) was used for all mask manipulations and PHASES (Furey, et al., PA33 Am. Cryst. Assoc. Mtg. Abstr. 18:73 (1990)) and the CCP4 suite (CCP4, 1994) were used for the generation of structure factors and the calculation of weights.

However, although the DES-LBD-GRIP1 NR Box II peptide complex model accounted for ~90% of the scattering matter in the asymmetric unit, refinement was being hampered by severe model bias. The OHT complex data set was then collected. Starting with one of the monomers of the preliminary DES-LBD model as the search probe, molecular replacement in AMoRe was used to search for the location of LBD in this crystal form in both $P6_122$ and $P6_522$. A translation search in $P6_522$ yielded the correct solution (R=53.8%, CC=38.2%). In order to reduce model bias, DMMULTI (CCP4, 1994) was then used to project averaged density from the DES complex cell into the OHT complex cell. Using MOLOC, a model of the LBD was built into the resulting density. The model was refined initially in REFMAC and later with the

simulated annealing, positional and B-factor refinement protocols in X-PLOR (Brunger, X-PLOR Version 3.843, New Haven, Connecticut: Yale University, 1996) using a maximum-likelihood target (Adams, et al., Proc. Natl. Acad. Sci. USA 94:5018-23 (1997)). Anisotropic scaling and a bulk solvent correction were used and all B-factors were refined isotropically. Except for the R_{free} set (a random sampling consisting of 8% of the data set), all data between 41 and 1.9Å (with no σ cutoff) were included. The final model consisted of residues 306-551, the ligand and 79 waters. According to PROCHECK (CCP4, 1994), 91.6% of all residues in the model were in the core regions of the Ramachandran plot and none were in the disallowed regions.

The high resolution data set of the DES-LBD-GRIP1 NR Box II peptide complex became available when the R_{free} of the OHT-LBD model was ~31%. Both monomers in the asymmetric unit of the DES complex crystal were relocated using AMoRe and the incompletely refined OHT-LBD model (with helix 12 and the loop between helices 11 and 12 removed) as the search model. The missing parts of the model were built and the rest of the model was corrected using MOLOC and two-fold averaged maps generated in DM. Initially, refinement was carried out with REFMAC using tight NCS restraints. At later stages, the model was refined without NCS restraints using the simulated annealing, positional and B-factor refinement protocols in X-PLOR and a maximum-likelihood target. All B-factors were refined isotropically and anisotropic scaling and a bulk solvent correction were used. The R_{free} set contained a random sample of 6.5% of all data. In refinement, all data between 27 and 2.03Å (with no σ cutoff) were used. The final model was composed of residues 305-549 of monomer A, residues 305-461 and 470-554 of monomer B, residues 687-697 of peptide A, residues 686-696 of peptide B, two ligand molecules, 147 waters, two carboxymethyl groups and a chloride ion. According to PROCHECK, 93.7% of all residues in the model were in the core regions of the Ramachandran plot and none were in the disallowed regions.

Figure 1A provides a view of a 2Fo-Fc electron density map calculated at 2.03Å resolution and contoured at 1.0 σ showing the GRIP1 NR box II interaction with the LBD. The GRIP1 NR Box II peptide (SEQ ID NO:4) was omitted from the model prior to map calculation. Ile 689 from the peptide and two of the three receptor residues with which it interacts (Glu 542 and Leu 539) are labeled. Asp 538 has been omitted for clarity. The hydrogen bonds between the γ-carboxylate of Glu 542 and the amides of residues 689 and 690 of the peptide are depicted as dashed orange bonds. Figure 1B provides a view of a 2Fo-Fc electron density map calculated

at 1.90Å resolution and contoured at 1.0 σ showing the N-terminal region of helix 12. The dashed orange bonds depict the water-mediated hydrogen bond network between the imidazole ring of His 377, the γ-carboxylate of Glu 380, and the amide of Tyr 537. The three labeled residues (Glu 380, Leu 536 and Tyr 537) interact with each other through van der Waals contacts and/or hydrogen bonds. Intriguingly, mutations in each these three residues dramatically increase the transcriptional activity of unliganded ERα LBD (Eng, et al., Mol. Cell. Biol. 17:4644-4653 (1997); Lazennec, et al., Mol. Endocrinol. 11:1375-86 (1997); White, et al., EMBO J. 16:1427-35 (1997)).

Example 2

Structure Determination

GRIP1, a mouse p160 coactivator, interacts both *in vivo* and *in vitro* with the ERα LBD bound to agonist (Ding, et al., supra), but not with the LBD bound to antagonist (Norris, et al., J. Biol. Chem. 273:6679-88 (1998)). Mutational studies of GRIP1 and its human homologue TIF2 suggest that of the three NR boxes from GRIP1, NR box II (residues 690 to 694) binds most tightly to the ERα LBD (Ding, et al., supra and Voegel, et al., supra).

Competition assays indicate that a 13 residue GRIP1 NR Box II peptide, NH_2-KHKILHRLLQDSS-CO_2H (SEQ ID NO:4), corresponding to residues 686-698 of GRIP1 (Ding, et al., supra), synthesized by standard solid phase methods, binds specifically to the agonist-bound ERα LBD (IC_{50}<0.4μM; Kushner, unpublished) and to other agonist-bound NR LBDs (Ding, et al., supra and Darimont, at al, supra).

An electrophoretic mobility shift assay was used to demonstrate that the GRIP1 NR Box II peptide (SEQ ID NO:4) bound the ERα LBD in the presence of the agonist, DES, but not the antagonist, OHT. Eight microgram samples of purified hERα-LBD bound to either DES or OHT were incubated in the absence of the GRIP1 NR Box II peptide (SEQ ID NO:4), i.e., buffer alone, or in the presence of either a 2-fold or 10-fold molar excess of the GRIP1 NR Box II peptide. The binding reactions were performed on ice for 45 minutes in 10 μl of buffer containing 20mM Tris, pH 8.1, 1mM DTT, and 200mM NaCl and then subjected to 6% native PAGE. Gels were stained with GELCODE Blue Stain reagent (Pierce).

In the presence of the NR box II peptide, the migration of the DES-LBD complex was retarded. In contrast, peptide addition had no effect on the mobility of the OHT-LBD complex. Hence, this peptide fragment of GRIP1 possesses the ligand-dependent receptor binding activity

characteristic of the full-length protein. These observations suggest that the GRIP1 NR Box II peptide is a valid model for studying the interaction between GRIP1 and the ERα LBD.

In order to characterize structurally the interaction between the GRIP1 NR Box II peptide and the ERα LBD, recombinant human ERα LBD (residues 297-554) was crystallized bound to both DES and the GRIP1 NR Box II peptide. The ERα LBD bound to OHT was also crystallized in order to determine the mechanism by which this antagonist blocks coactivator/ERα interaction. X-ray diffraction data from these crystals were measured and the structures were determined by a combination of molecular replacement (using a modified version of the coordinates of the human retinoic acid receptor γ (RARγ) LBD, Renaud, et al., supra, as the search model) and aggressive density modification.

The structure of the DES-ERα LBD-GRIP1 NR Box II peptide complex has been refined to a crystallographic R-factor of 19.9% (R_{free}=25.0%) using data to 2.03Å resolution, as shown in Figure 1A and Table 2. The structure of the OHT-ERα LBD complex has been refined using data to 1.90Å to a crystallographic R-factor of 23.0% (R_{free}=26.2%), as shown in Figure 1B and Table 2.

Table 2
Summary of Crystallographic Statistics

	Ligand	
Data Collection	DES	OHT
Space group	$P2_1$	$P6_522$
Resolution	2.03	1.90
Observations	104189	269253
Unique	30265	23064
Completeness (%)	98.4	99.1
R_{sym}(%)[a]	7.8	7.0
Average I/σI	9.8	16.1
Refinement		
Number of non-hydrogen atoms	4180	2070
R_{cryst} (%)[b]/R_{free} (%)	19.9/25.0	23.0/26.1
Bond r.m.s. deviation (Å)	0.006	0.006
Angle r.m.s. deviation (°)	1.05	1.05
Average B factor (Å^2)	34.0	40.4

[a] $R_{sym} = \sum_i | I_i - \langle I_i \rangle | / \sum_i I_i$ where $\langle I_i \rangle$ is the average intensity over symmetry equivalents

[b] $R_{cryst} = \sum | F_o - F_c | / \sum | F_o |$

Example 3

Overall Structure of the DES-LBD-GRIP1 NR Box II Peptide Complex

The asymmetric unit of the DES-LBD-GRIP1 NR Box II peptide complex crystals contains the same noncrystallographic dimer of LBDs that has been observed in the previously determined structures of the LBD bound to both E_2 and RAL (Brzozowski, et al., supra and Tanenbaum, et al., supra). Beyond the flexible loops between helices 2 and 3 and helices 9 and 10, the two LBDs of the dimer adopt similar structures (r.m.s.d. 0.47Å based on Cα positions). The conformation of each LBD complexed with DES closely resembles that of the LBD bound to E_2 (Brzozowski, et al., supra); each monomer is a wedge shaped molecule consisting of three layers of eleven to twelve helices and a single beta hairpin (Figure 2A). In each LBD, the hydrophobic face of helix 12 is packed against helices 3, 5/6 and 11 covering the ligand binding pocket (Figure 2A). One GRIP1 NR Box II peptide is bound to each LBD in a hydrophobic cleft composed of residues from helices 3, 4, 5 and 12 and the turn between 3 and 4 (Figures 2A and 3A). The density for both peptides in the asymmetric unit is continuous and unambiguous (Figure 1A). Residues 687 to 697 from the GRIP1 NR Box II peptide, designated peptide A, and residues 686 to 696 from the GRIP1 NR Box II peptide, designated peptide B, have been modeled; the remaining residues are disordered. Given that each peptide lies within a different environment within the crystal, it is striking that from residues Ile 689 to Gln 695 each peptide forms a two turn, amphipathic α helix (Figures 2A and 3A). Flanking this region of common secondary structure, the peptides adopt dissimilar random coil conformations.

The overall structures of the DES-ERα LBD-GRIP1 NR Box II peptide complex and the OHT-ERα LBD complex are illustrated in Figure 2. In Figure 2A, the coactivator peptide and the LBD are shown as ribbon drawings. The peptide is colored gold and helix 12 (residues 538-546) is colored magenta. Helices 3, 4 and 5 (labeled H3, H4 and H5 respectively) are colored blue. DES, colored green, is shown in space-filling representation. In Figure 2B, the LBD is depicted as a ribbon drawing. As in Figure 2A, helix 12 (residues 536-544) is colored in magenta and helices 3, 4 and 5 are colored blue. OHT, in red, is shown in space-filling representation.

Example 4

The NR Box II Peptide-LBD Interface

The binding of the GRIP1 NR Box II peptide to the ERα LBD buries 1000Å^2 of predominantly hydrophobic surface area from both molecules. The GRIP1 NR Box II peptide binding site is a shallow groove composed of residues Leu 354, Val 355, Ile 358, Ala 361 and

Lys 362 from helix 3; Phe 367 and Val 368 from helix 4; Leu 372 from the turn between helices 3 and 4; Gln 375, Val 376, Leu 379 and Glu 380 from helix 5; and Asp 538, Leu 539, Glu 542 and Met 543 from helix 12 (Figure 3A). The floor and sides of this groove are completely nonpolar, but the ends of this groove are charged (Figure 3C).

The LBD interacts primarily with the hydrophobic face of the GRIP1 NR Box II peptide α helix formed by the side chains of Ile 689 and the three LXXLL motif (SEQ ID NO:1) leucines (Leu 690, Leu 693 and Leu 694). The side chain of Leu 690 is deeply embedded within the groove and forms van der Waals contacts with the side chains of Ile 358, Val 376, Leu 379, Glu 380 and Met 543 (Figure 3A and 3C). The side chain of Leu 694 is similarly isolated within the groove and makes van der Waals contacts with the side chains of Ile 358, Lys 362, Leu 372, Gln 375, Val 376 and Leu 379 (Figure 3A and 3C). In contrast, the side chains of both Ile 689 and the second NR box leucine, Leu 693, rest against the rim of the groove (Figure 3A and 3C). The side chain of Ile 689 lies in a shallow depression formed by the side chains of Asp 538, Leu 539 and Glu 542. The side chain of Leu 693 makes nonpolar contacts with the side chains of Ile 358 and Leu 539.

The charged and polar side chains which form the hydrophilic face of the peptide helix project away from the receptor and either interact predominantly with solvent or form symmetry contacts (Figure 1A). None of the side chains of the polar and charged residues outside the helical region of either peptide in the asymmetric unit, with the exception of Lys 688 of peptide B, is involved in hydrogen bonds or salt bridges with its associated LBD monomer. The ε-amino group of Lys 688 of peptide B hydrogen bonds to the side chain carboxylate of Glu 380 of monomer B. This interaction is presumably a crystal artifact; the main chain atoms of the N-terminal three residues of peptide B are displaced from monomer B and interact extensively with a symmetry-related LBD.

In addition to interacting with the hydrophobic face of the peptide helix, the LBD stabilizes the main chain conformation of the NR box peptide by forming capping interactions with both ends of the peptide helix. Glu 542 and Lys 362 are positioned at opposite ends of the peptide binding site (Figure 3A). The side chains of Glu 542 and Lys 362 form van der Waals contacts with main chain and side chain atoms at the N- and C-terminal turns of the peptide helix respectively . These interactions position the stabilizing charges of the γ-carboxylate of Glu 542 and ε-amino group of Lys 362 near the ends of the GRIP1 NR Box II peptide helix (Figure 3C). The side chain carboxylate (γ-carboxylate) of Glu 542 hydrogen bonds to the amides of the

residues of N-terminal turn of the peptide helix (residues 688 and 689 of peptide A; residues 689 and 690 of peptide B) (Figure 1A). Similarly, the ε-amino group of Lys 362 hydrogen bonds to the carbonyls of the residues of the C-terminal turn of the peptide helix (residue 693 of peptide A; residues 693 and 694 of peptide B) (Figure 5).

To test the importance of the GRIP1 NR Box II peptide/LBD interface observed in the crystal, a series of site-directed mutations were introduced into the ERα LBD. These mutations were designed either to simultaneously perturb the structural integrity and the nonpolar character of the floor of the binding groove (Ile 358->Arg, Val 376->Arg and Leu 539->Arg) or to prevent the formation of the capping interactions (Lys 362->Ala and Glu 542->Lys). Fusions of glutathione-S-transferase (GST) to the wild-type and mutant LBDs were analyzed for their ability to bind ^{35}S-labeled GRIP1 in the absence of ligand or in the presence of DES or OHT.

^{35}S-labeled GRIP1 was incubated with either immobilized GST, immobilized wild type GST-hERα LBD, or immobilized mutant GST-LBDs in the absence of ligand or in the presence of DES or OHT. The bound GRIP1 was quantitated after SDS-PAGE. I358R, mutant LBD containing a Ile->Arg substitution at residue 358; K362A, mutant LBD containing a Lys->Ala substitution at residue 362; V376R, mutant LBD containing a Val->Arg substitution at residue 376; L539R, mutant LBD containing a Leu->Arg substitution at residue 539; E542K, mutant LBD containing a Glu->Lys substitution at residue 542.

In the absence of ligand or in the presence of OHT, fusions to the wild-type protein and all of the mutant LBDs showed no detectable binding to GRIP1. The Ile 358->Arg, Val 376->Arg and Leu 539->Arg mutants were all unable to interact with coactivator in the presence of agonist, confirming the importance of the packing interactions observed in the crystal. Disruption of either the N- or C-terminal capping interaction also compromised GRIP1 binding in the presence of agonist. Only the wild-type GST-LBD was able to recognize the coactivator in the presence of DES.

Example 5
Agonist Recognition

Despite its different shape and larger molecular volume, DES (273Å^3) is accommodated within the same binding pocket that recognizes E_2 (252Å^3). In its receptor complex, DES is completely encased within the narrower half of the LBD in a predominantly hydrophobic cavity composed of residues from helices 3, 6, 7, 8, 11, and 12 as well as the S1/S2 hairpin (Figures 2A and 4A).

The interaction of DES with ERα resembles that of E_2. One of the phenolic rings of DES lies in the same position as the E_2 A ring near helices 3 and 6. Like the aromatic ring of the E_2, the DES A ring (Figure 4A) is engaged by the side chains of Phe 404, Ala 350, Leu 387 and Leu 391 with its phenolic hydroxyl forming hydrogen bonds to the γ-carboxylate of Glu 353, to the guanidinium group of Arg 394, and to a structurally conserved water molecule. The A' ring of DES (Figure 4A) is bound near helices 7, 8 and 11 adjacent to the location of the E_2 C and D rings. This ring forms van der Waals contacts not only with Gly 521 and Leu 525, like the D ring of E_2, but also with Met 343, Leu 346 and Met 421 (Figure 4A). Even though it is located 1.7Å from the position of the D ring hydroxyl, the DES A' ring phenolic hydroxyl is still able to hydrogen bond to the imidazole ring of His 524 (Figure 4A).

DES also forms contacts with the LBD that E_2 does not. There are unoccupied cavities adjacent to the α face of the B ring and the β face of the C ring of the E_2 (Brzozowski, et al., supra and Tanenbaum, et al., supra). The ethyl groups of DES, which project perpendicularly from the plane of the phenolic rings, fit snugly into these spaces. The resulting additional nonpolar contacts with the side chains of Ala 350, Leu 384, Phe 404, and Leu 428 (Figure 4A) may account for the higher affinity of DES for the receptor (Kuiper, et al., Endocrinology 138:863-70 (1997)).

Except for Met 421 and Met 528 (both of which contact only DES) and Met 388 and Ile 424 (both of which contact only E_2), the ER is able to use the same residues to form all of the observed hydrogen bonds and van der Waals contacts with both agonists (Figure 4A, Brzozowski, et al., supra, and Tanenbaum, et al., supra). This remarkable adaptability is presumably the result of both relatively large molecular volume of the binding pocket (~500Å^3 in both complexes) and its apparent structural plasticity. In particular, at the DES A' ring/steroid D ring end of the binding pocket, Met 343, Met 421, His 524 and Met 528 adopt different packing configurations in response to each ligand (data not shown). This plasticity may be necessary to allow the receptor to recognize endogenous estrogens such as estrone and estriol, which differ structurally from E_2 at the D ring.

Example 6

Structure of the OHT-LBD Complex

The binding of OHT induces a conformation of the LBD that differs in both secondary and tertiary structural organization from that driven by DES binding. In the DES complex, the main chain from residues 339 to 341, 421 to 423, and 527 to 530 form parts of helices 3, 8 and

11 respectively. In contrast, these regions adopt an extended conformation in the OHT complex (Figures 2A, 2B and 6A). In addition, the composition and orientation of helix 12 are different in the two structures. Helix 12 in the DES complex consists of residues 538 to 546 whereas helix 12 in the OHT complex consists of residues 536 to 544. Most dramatically, rather than covering the ligand binding pocket as it does in the DES complex, helix 12 in the OHT complex occupies the part of the coactivator binding groove formed by residues from helices 3, 4, and 5, and the turn connecting helices 3 and 4 (Figures 2A, 2B and 3B). This alternative conformation of helix 12 appears to be similar to that observed in the RAL complex (Brzozowski, et al., supra).

Example 7
Helix 12-LBD Interface

Except for the orientation of helix 12, the structure of the peptide binding groove is almost identical in the DES and OHT complexes (Figures 3A and 3B). The region of this groove outside of helix 12 is referred to herein as the "static region" of the NR box binding site. Helix 12 in the OHT complex and the NR box peptide helix in the DES complex interact with the static region of the coactivator recognition groove in strikingly similar ways.

Helix 12 mimics the hydrophobic interactions of the NR box peptide with the static region of the groove with a stretch of residues (residues 540 to 544) that resembles an NR box (LLEML instead of LXXLL) (SEQ ID NO:3 instead of SEQ ID NO:1). The side chains of Leu 540 and Met 543 lie in approximately the same locations as those of the first and second motif leucines (Leu 690 and Leu 693) in the peptide complex (Figure 5). Leu 540 is inserted into the groove and makes van der Waals contacts with Leu 354, Val 376 and Glu 380 (Figures 3B and 3D). Met 543 lies along the edge of the groove and forms van der Waals contacts with the side chains of Leu 354, Val 355 and Ile 358 (Figures 3B and 3D). The side chain position of Leu 544 almost exactly overlaps that of the third NR box leucine, Leu 694 (Figure 5). Deep within the groove, the Leu 544 side chain makes van der Waals contacts with the side chains of Ile 358, Lys 362, Leu 372, Gln 375, Val 376 and Leu 379 (Figures 3B and 3D).

Helix 12 in the OHT complex is also stabilized by N- and C-terminal capping interactions. Lys 362 interacts with the C-terminal turn of helix 12 much as it does with the equivalent turn of the peptide helix (Figures 3A and 3B). The Lys 362 side chain packs against the C-terminal turn of the helix 12 with its ε-amino group hydrogen bonding to the carbonyls of residues 543 and 544 (Figure 5). Given that the capping interaction at the N-terminal turn coactivator helix is formed by a helix 12 residue (Glu 542), the N-terminal turn of helix 12 in the

antagonist complex is forced to interact with another residue, Glu 380 (Figures 3B and 3D). The Glu 380 γ-carboxylate forms van der Waals contacts with Tyr 537 and interacts with the amide of Tyr 537 through a series of water-mediated hydrogen bonds (Figure 1B).

In addition to forming these "NR box-like" interactions, helix 12 also forms van der Waals contacts with areas of the LBD outside of the coactivator recognition groove. The side chain of Leu 536 forms van der Waals contacts with Glu 380 and Trp 383 and that of Tyr 537 forms van der Waals contacts with His 373, Val 376 and Glu 380 (Figures 1B, 3B and 3D). As a result of these contacts, helix 12 in the OHT complex buries more solvent accessible surface area (~1200Å^2) than the NR box peptide in the DES complex.

Example 8
OHT Recognition

OHT is bound within the same pocket that recognizes DES, E_2 and RAL. The orientation of OHT within the binding pocket appears to be dictated by the positioning of two structural features of this ligand, the phenolic A ring and the bulky side chain (Figures 4B and 6C). The A ring of OHT is bound in approximately the same location as the A ring of DES near helices 3 and 6 with its phenolic hydroxyl hydrogen bonding to a structurally conserved water and to the side chains of Glu 353 and Arg 394 (Figure 4B). Like the bulky side chain of RAL, the side chain of OHT exits the binding pocket between helices 3 and 11 (Figures 2B and 4B). The OHT C ring (Figure 4B) forms van der Waals contacts with the side chains of Met 343, Leu 346, Thr 347, Ala 350, Trp 383, Leu 384, Leu 387 and Leu 525. The positioning of the flexible dimethylaminoethyl region of the side chain is stabilized by van der Waals contacts with Thr 347, Ala 350 and Trp 383 and by a salt-bridge between the dimethylamino group of the side chain and the β-carboxylate of Asp 351, which lies 3.8Å away (Figure 4B). The positions of the A ring and the side chain in the context of the rigid triphenylethylene framework of OHT requires that the ethylene group of OHT lie in an orientation nearly orthogonal to that of the ethylene group of DES (Figures 4A, 4B and 6D). As a result, the B ring of OHT is driven more deeply into the binding pocket than the A' ring of DES (Figures 6B and 6C).

This location of the OHT B ring apparently cannot be accommodated by the same mechanisms that allow the DES A' ring/E_2 D ring end of the binding pocket to adapt to the different structural features of DES and E_2. Instead, the residues that contact the B ring (Met 343, Leu 346, Met 421, Ile 424, Gly 521, His 524 and Leu 525), most of which also interact with the A' ring of DES, adopt conformations distinct from the ones they adopt in the DES structure (Figure 6D). In fact, the location of the B ring actually precludes the side chain of one residue,

Met 421, from adopting the same conformation that it adopts in the DES structure (Figures 6B and 6C). As a consequence of these B ring-induced side chain conformations, many interresidue van der Waals contacts present in the DES complex are absent in the OHT complex. For example, whereas Met 421 packs against His 524 from helix 11 and against Met 343 from helix 3 in the agonist complexes, it is precluded by the location of the OHT B ring from interacting with either of these residues in the antagonist complex (Figure 6D).

The structural effects of the placement of the B ring are not limited to the residues that contact the B ring; the conformations of these residues force other residues throughout the binding pocket to, in turn, adopt alternative conformations. For instance, the conformation adopted by Met 421 in the OHT complex prevents the side chains of Phe 404 and Phe 425 from occupying the positions they take in the DES complex (Figure 6B and 6C). As a consequence, Phe 404 does not make van der Waals contacts with the OHT A ring as it does with the A rings of DES or E_2 (Figure 6C). In fact, Phe 404 only contacts the ethyl group of OHT (Figures 6C and 6D). The alternative conformations of the side chains of both the residues that directly contact the B ring and those that are indirectly affected by it, force the main chain throughout the binding pocket to adopt a different conformation as well (Figure 6D).

Identification and characterization of key residues within ligand binding domain of the ERα and extension of this information to other nuclear receptors shows that these residues are common for all nuclear receptors identified to date. Thus, the Examples presented herein demonstrate that information derived from the structure and function of the ERα ligand binding domain can be applied in design and selection of compounds that modulate binding of compounds to nuclear receptors for all members of the nuclear receptor family.

All publications and patent applications mentioned in this specification are herein incorporated by reference to the same extent as if each individual publication or patent application was specifically and individually indicated to be incorporated by reference.

The invention now being fully described, it will be apparent to one of ordinary skill in the art that many changes and modifications can be made thereto without departing from the spirit or scope of the appended claims.

Appendix 1

Atomic Coordinates for Human ERα Complexed With DES and a GRIP1 NR Box II Peptide

CRYST1	54.094	82.217	58.041	90.00	111.33	90.00	P 21	2		
ORIGX1	1.000000	0.000000	0.000000	0.00000						
ORIGX2	0.000000	1.000000	0.000000	0.00000						
ORIGX3	0.000000	0.000000	1.000000	0.00000						
SCALE1	0.018486	0.000000	0.007221	0.00000						
SCALE2	0.000000	0.012163	0.000000	0.00000						
SCALE3	0.000000	0.000000	0.018497	0.00000						
ATOM	1	CB	SER	A	305	35.230	-14.787	-1.163	1.00	73.26
ATOM	2	C	SER	A	305	35.331	-14.303	1.289	1.00	72.95
ATOM	3	O	SER	A	305	34.146	-13.984	1.186	1.00	72.46
ATOM	4	N	SER	A	305	36.797	-16.033	0.285	1.00	74.06
ATOM	5	CA	SER	A	305	36.138	-14.713	0.061	1.00	73.59
ATOM	6	N	LEU	A	306	35.982	-14.313	2.449	1.00	72.21
ATOM	7	CA	LEU	A	306	35.329	-13.950	3.702	1.00	71.05
ATOM	8	CB	LEU	A	306	36.251	-14.256	4.878	1.00	70.19
ATOM	9	C	LEU	A	306	34.929	-12.478	3.719	1.00	69.57
ATOM	10	O	LEU	A	306	35.580	-11.638	3.100	1.00	69.96
ATOM	11	N	ALA	A	307	33.851	-12.176	4.434	1.00	68.06
ATOM	12	CA	ALA	A	307	33.358	-10.810	4.541	1.00	64.88
ATOM	13	CB	ALA	A	307	31.841	-10.795	4.436	1.00	65.83
ATOM	14	C	ALA	A	307	33.792	-10.204	5.866	1.00	63.36
ATOM	15	O	ALA	A	307	33.878	-8.984	6.005	1.00	62.73
ATOM	16	N	LEU	A	308	34.064	-11.062	6.842	1.00	62.52
ATOM	17	CA	LEU	A	308	34.487	-10.598	8.156	1.00	62.57
ATOM	18	CB	LEU	A	308	34.423	-11.745	9.171	1.00	62.81
ATOM	19	CG	LEU	A	308	33.214	-12.688	9.130	1.00	64.21
ATOM	20	CD1	LEU	A	308	33.188	-13.513	10.406	1.00	66.28
ATOM	21	CD2	LEU	A	308	31.919	-11.898	8.989	1.00	63.80
ATOM	22	C	LEU	A	308	35.903	-10.037	8.100	1.00	61.61
ATOM	23	O	LEU	A	308	36.385	-9.445	9.066	1.00	62.92
ATOM	24	N	SER	A	309	36.561	-10.219	6.959	1.00	60.50
ATOM	25	CA	SER	A	309	37.928	-9.743	6.771	1.00	58.73
ATOM	26	CB	SER	A	309	38.720	-10.750	5.934	1.00	59.53
ATOM	27	OG	SER	A	309	38.889	-10.283	4.606	1.00	59.47
ATOM	28	C	SER	A	309	37.986	-8.373	6.099	1.00	57.05
ATOM	29	O	SER	A	309	38.965	-7.637	6.249	1.00	56.70
ATOM	30	N	LEU	A	310	36.940	-8.038	5.352	1.00	52.69
ATOM	31	CA	LEU	A	310	36.877	-6.759	4.658	1.00	48.20
ATOM	32	CB	LEU	A	310	35.516	-6.596	3.974	1.00	48.32
ATOM	33	CG	LEU	A	310	35.301	-7.188	2.583	1.00	44.94
ATOM	34	CD1	LEU	A	310	33.951	-6.728	2.055	1.00	46.45
ATOM	35	CD2	LEU	A	310	36.417	-6.755	1.650	1.00	43.19

ATOM	36	C	LEU	A	310	37.086	-5.589	5.609	1.00	46.44
ATOM	37	O	LEU	A	310	36.605	-5.607	6.741	1.00	46.78
ATOM	38	N	THR	A	311	37.812	-4.576	5.148	1.00	44.36
ATOM	39	CA	THR	A	311	38.034	-3.380	5.949	1.00	42.88
ATOM	40	CB	THR	A	311	39.313	-2.633	5.532	1.00	42.31
ATOM	41	OG1	THR	A	311	39.079	-1.936	4.303	1.00	42.50
ATOM	42	CG2	THR	A	311	40.464	-3.606	5.350	1.00	46.02
ATOM	43	C	THR	A	311	36.834	-2.475	5.674	1.00	43.21
ATOM	44	O	THR	A	311	36.021	-2.776	4.800	1.00	42.12
ATOM	45	N	ALA	A	312	36.726	-1.372	6.409	1.00	42.16
ATOM	46	CA	ALA	A	312	35.616	-0.444	6.228	1.00	40.10
ATOM	47	CB	ALA	A	312	35.741	0.709	7.205	1.00	40.07
ATOM	48	C	ALA	A	312	35.561	0.090	4.799	1.00	41.80
ATOM	49	O	ALA	A	312	34.510	0.074	4.154	1.00	37.81
ATOM	50	N	ASP	A	313	36.698	0.564	4.304	1.00	42.35
ATOM	51	CA	ASP	A	313	36.752	1.104	2.953	1.00	42.27
ATOM	52	CB	ASP	A	313	38.133	1.703	2.680	1.00	43.74
ATOM	53	CG	ASP	A	313	38.323	3.054	3.348	1.00	46.62
ATOM	54	OD1	ASP	A	313	39.414	3.645	3.205	1.00	51.01
ATOM	55	OD2	ASP	A	313	37.380	3.529	4.015	1.00	48.89
ATOM	56	C	ASP	A	313	36.422	0.027	1.926	1.00	38.68
ATOM	57	O	ASP	A	313	35.704	0.281	0.959	1.00	38.75
ATOM	58	N	GLN	A	314	36.931	-1.179	2.145	1.00	34.76
ATOM	59	CA	GLN	A	314	36.666	-2.277	1.229	1.00	33.55
ATOM	60	CB	GLN	A	314	37.462	-3.512	1.643	1.00	36.90
ATOM	61	CG	GLN	A	314	38.963	-3.384	1.436	1.00	40.45
ATOM	62	CD	GLN	A	314	39.700	-4.610	1.905	1.00	43.13
ATOM	63	OE1	GLN	A	314	39.394	-5.196	2.935	1.00	43.60
ATOM	64	NE2	GLN	A	314	40.701	-5.032	1.117	1.00	44.03
ATOM	65	C	GLN	A	314	35.176	-2.595	1.201	1.00	34.95
ATOM	66	O	GLN	A	314	34.605	-2.860	0.140	1.00	32.89
ATOM	67	N	MET	A	315	34.542	-2.564	2.374	1.00	32.54
ATOM	68	CA	MET	A	315	33.115	-2.848	2.470	1.00	35.46
ATOM	69	CB	MET	A	315	32.650	-2.794	3.926	1.00	37.09
ATOM	70	CG	MET	A	315	31.137	-2.777	4.097	1.00	39.42
ATOM	71	SD	MET	A	315	30.443	-4.426	4.053	1.00	46.55
ATOM	72	CE	MET	A	315	31.351	-5.205	5.397	1.00	45.29
ATOM	73	C	MET	A	315	32.311	-1.859	1.640	1.00	31.83
ATOM	74	O	MET	A	315	31.453	-2.247	0.852	1.00	32.10
ATOM	75	N	VAL	A	316	32.587	-0.560	1.830	1.00	32.62
ATOM	76	CA	VAL	A	316	31.882	0.470	1.079	1.00	31.09
ATOM	77	CB	VAL	A	316	32.395	1.888	1.425	1.00	34.77
ATOM	78	CG1	VAL	A	316	31.786	2.899	0.461	1.00	34.10
ATOM	79	CG2	VAL	A	316	32.021	2.246	2.862	1.00	34.40
ATOM	80	C	VAL	A	316	32.092	0.232	-0.414	1.00	33.48
ATOM	81	O	VAL	A	316	31.145	0.266	-1.200	1.00	32.49
ATOM	82	N	SER	A	317	33.337	-0.027	-0.795	1.00	33.49
ATOM	83	CA	SER	A	317	33.682	-0.280	-2.187	1.00	32.88

ATOM	84	CB	SER	A	317	35.165	-0.635	-2.297	1.00	35.77
ATOM	85	OG	SER	A	317	35.825	0.277	-3.154	1.00	42.70
ATOM	86	C	SER	A	317	32.849	-1.396	-2.801	1.00	30.71
ATOM	87	O	SER	A	317	32.279	-1.238	-3.880	1.00	31.14
ATOM	88	N	ALA	A	318	32.792	-2.529	-2.111	1.00	29.51
ATOM	89	CA	ALA	A	318	32.035	-3.676	-2.580	1.00	29.93
ATOM	90	CB	ALA	A	318	32.156	-4.811	-1.579	1.00	28.56
ATOM	91	C	ALA	A	318	30.565	-3.305	-2.771	1.00	31.55
ATOM	92	O	ALA	A	318	29.961	-3.642	-3.784	1.00	30.64
ATOM	93	N	LEU	A	319	29.997	-2.614	-1.791	1.00	34.13
ATOM	94	CA	LEU	A	319	28.597	-2.212	-1.861	1.00	32.93
ATOM	95	CB	LEU	A	319	28.170	-1.576	-0.540	1.00	31.15
ATOM	96	CG	LEU	A	319	28.076	-2.555	0.632	1.00	32.27
ATOM	97	CD1	LEU	A	319	27.523	-1.840	1.852	1.00	32.14
ATOM	98	CD2	LEU	A	319	27.194	-3.733	0.243	1.00	31.82
ATOM	99	C	LEU	A	319	28.340	-1.257	-3.020	1.00	34.41
ATOM	100	O	LEU	A	319	27.430	-1.475	-3.818	1.00	35.23
ATOM	101	N	LEU	A	320	29.140	-0.195	-3.120	1.00	32.53
ATOM	102	CA	LEU	A	320	28.972	0.756	-4.212	1.00	35.33
ATOM	103	CB	LEU	A	320	30.052	1.839	-4.155	1.00	33.52
ATOM	104	CG	LEU	A	320	29.974	2.899	-3.054	1.00	34.60
ATOM	105	CD1	LEU	A	320	31.060	3.940	-3.292	1.00	33.69
ATOM	106	CD2	LEU	A	320	28.611	3.562	-3.044	1.00	31.05
ATOM	107	C	LEU	A	320	29.052	0.040	-5.561	1.00	35.41
ATOM	108	O	LEU	A	320	28.230	0.271	-6.446	1.00	39.16
ATOM	109	N	AASP	A	321	30.042	-0.833	-5.720	0.50	36.33
ATOM	110	N	BASP	A	321	30.041	-0.839	-5.695	0.50	35.76
ATOM	111	CA	AASP	A	321	30.214	-1.559	-6.977	0.50	37.71
ATOM	112	CA	BASP	A	321	30.258	-1.595	-6.925	0.50	37.11
ATOM	113	CB	AASP	A	321	31.537	-2.334	-6.973	0.50	40.01
ATOM	114	CB	BASP	A	321	31.573	-2.374	-6.826	0.50	39.41
ATOM	115	CG	AASP	A	321	31.694	-3.230	-8.195	0.50	41.93
ATOM	116	CG	BASP	A	321	32.770	-1.562	-7.284	0.50	39.96
ATOM	117	OD1	AASP	A	321	31.523	-2.733	-9.329	0.50	42.11
ATOM	118	OD1	BASP	A	321	33.312	-1.868	-8.366	0.50	43.41
ATOM	119	OD2	AASP	A	321	31.988	-4.432	-8.022	0.50	42.69
ATOM	120	OD2	BASP	A	321	33.170	-0.622	-6.564	0.50	41.33
ATOM	121	C	AASP	A	321	29.069	-2.524	-7.275	0.50	37.19
ATOM	122	C	BASP	A	321	29.123	-2.565	-7.253	0.50	36.68
ATOM	123	O	AASP	A	321	28.820	-2.861	-8.434	0.50	36.87
ATOM	124	O	BASP	A	321	28.934	-2.942	-8.411	0.50	36.08
ATOM	125	N	ALA	A	322	28.374	-2.968	-6.235	1.00	35.35
ATOM	126	CA	ALA	A	322	27.268	-3.902	-6.417	1.00	31.59
ATOM	127	CB	ALA	A	322	27.124	-4.781	-5.175	1.00	30.73
ATOM	128	C	ALA	A	322	25.946	-3.204	-6.709	1.00	30.07
ATOM	129	O	ALA	A	322	24.955	-3.857	-7.036	1.00	26.53
ATOM	130	N	GLU	A	323	25.932	-1.880	-6.596	1.00	27.98
ATOM	131	CA	GLU	A	323	24.713	-1.117	-6.827	1.00	29.88

	ATOM	132	CB	GLU	A	323	25.027	0.380	-6.855	1.00	30.98
	ATOM	133	CG	GLU	A	323	24.870	1.068	-5.509	1.00	31.62
	ATOM	134	CD	GLU	A	323	23.463	0.940	-4.960	1.00	31.98
	ATOM	135	OE1	GLU	A	323	23.183	-0.056	-4.257	1.00	33.10
5	ATOM	136	OE2	GLU	A	323	22.640	1.836	-5.233	1.00	30.01
	ATOM	137	C	GLU	A	323	24.010	-1.515	-8.123	1.00	30.86
	ATOM	138	O	GLU	A	323	24.655	-1.705	-9.151	1.00	28.86
	ATOM	139	N	PRO	A	324	22.674	-1.659	-8.083	1.00	30.66
	ATOM	140	CD	PRO	A	324	21.774	-1.466	-6.935	1.00	31.01
10	ATOM	141	CA	PRO	A	324	21.935	-2.032	-9.290	1.00	30.29
	ATOM	142	CB	PRO	A	324	20.613	-2.598	-8.760	1.00	31.42
	ATOM	143	CG	PRO	A	324	20.626	-2.363	-7.258	1.00	33.66
	ATOM	144	C	PRO	A	324	21.717	-0.785	-10.138	1.00	27.46
	ATOM	145	O	PRO	A	324	21.893	0.332	-9.668	1.00	26.19
15	ATOM	146	N	PRO	A	325	21.335	-0.959	-11.403	1.00	27.80
	ATOM	147	CD	PRO	A	325	21.082	-2.198	-12.161	1.00	27.35
	ATOM	148	CA	PRO	A	325	21.125	0.242	-12.211	1.00	25.59
	ATOM	149	CB	PRO	A	325	21.258	-0.266	-13.637	1.00	24.02
	ATOM	150	CG	PRO	A	325	20.773	-1.695	-13.559	1.00	26.00
20	ATOM	151	C	PRO	A	325	19.749	0.830	-11.954	1.00	23.73
	ATOM	152	O	PRO	A	325	18.873	0.165	-11.402	1.00	24.83
	ATOM	153	N	ILE	A	326	19.571	2.081	-12.352	1.00	22.11
	ATOM	154	CA	ILE	A	326	18.296	2.762	-12.212	1.00	24.01
	ATOM	155	CB	ILE	A	326	18.502	4.282	-12.133	1.00	25.97
25	ATOM	156	CG2	ILE	A	326	17.168	4.992	-12.286	1.00	20.75
	ATOM	157	CG1	ILE	A	326	19.189	4.632	-10.805	1.00	29.31
	ATOM	158	CD1	ILE	A	326	19.301	6.120	-10.525	1.00	32.91
	ATOM	159	C	ILE	A	326	17.506	2.408	-13.471	1.00	25.72
	ATOM	160	O	ILE	A	326	17.906	2.758	-14.581	1.00	25.55
30	ATOM	161	N	LEU	A	327	16.392	1.703	-13.301	1.00	25.57
	ATOM	162	CA	LEU	A	327	15.595	1.279	-14.439	1.00	23.80
	ATOM	163	CB	LEU	A	327	14.872	-0.029	-14.104	1.00	23.96
	ATOM	164	CG	LEU	A	327	15.778	-1.210	-13.728	1.00	19.89
	ATOM	165	CD1	LEU	A	327	14.944	-2.462	-13.583	1.00	21.19
35	ATOM	166	CD2	LEU	A	327	16.850	-1.415	-14.805	1.00	17.53
	ATOM	167	C	LEU	A	327	14.598	2.317	-14.935	1.00	27.16
	ATOM	168	O	LEU	A	327	14.161	3.202	-14.194	1.00	25.98
	ATOM	169	N	TYR	A	328	14.251	2.207	-16.210	1.00	26.56
	ATOM	170	CA	TYR	A	328	13.303	3.123	-16.814	1.00	24.45
40	ATOM	171	CB	TYR	A	328	13.724	3.465	-18.245	1.00	26.72
	ATOM	172	CG	TYR	A	328	14.587	4.693	-18.314	1.00	27.73
	ATOM	173	CD1	TYR	A	328	14.021	5.949	-18.518	1.00	28.56
	ATOM	174	CE1	TYR	A	328	14.798	7.092	-18.509	1.00	29.10
	ATOM	175	CD2	TYR	A	328	15.962	4.612	-18.110	1.00	26.01
45	ATOM	176	CE2	TYR	A	328	16.750	5.753	-18.098	1.00	30.63
	ATOM	177	CZ	TYR	A	328	16.157	6.988	-18.297	1.00	30.07
	ATOM	178	OH	TYR	A	328	16.917	8.130	-18.265	1.00	37.94
	ATOM	179	C	TYR	A	328	11.923	2.501	-16.827	1.00	24.95

	ATOM	180	O	TYR	A	328	11.774	1.274	-16.846	1.00	27.02
	ATOM	181	N	SER	A	329	10.912	3.358	-16.800	1.00	25.60
	ATOM	182	CA	SER	A	329	9.533	2.908	-16.837	1.00	29.45
	ATOM	183	CB	SER	A	329	8.661	3.858	-16.020	1.00	30.80
5	ATOM	184	OG	SER	A	329	7.297	3.721	-16.364	1.00	33.74
	ATOM	185	C	SER	A	329	9.129	2.947	-18.313	1.00	31.30
	ATOM	186	O	SER	A	329	9.908	3.397	-19.154	1.00	27.35
	ATOM	187	N	GLU	A	330	7.930	2.469	-18.629	1.00	32.98
	ATOM	188	CA	GLU	A	330	7.459	2.482	-20.007	1.00	35.10
10	ATOM	189	CB	GLU	A	330	6.031	1.968	-20.074	1.00	34.67
	ATOM	190	C	GLU	A	330	7.532	3.924	-20.505	1.00	40.06
	ATOM	191	O	GLU	A	330	7.068	4.841	-19.826	1.00	42.65
	ATOM	192	N	TYR	A	331	8.124	4.126	-21.681	1.00	41.16
	ATOM	193	CA	TYR	A	331	8.263	5.470	-22.234	1.00	42.66
15	ATOM	194	CB	TYR	A	331	9.323	5.482	-23.350	1.00	42.54
	ATOM	195	CG	TYR	A	331	9.202	4.347	-24.345	1.00	38.67
	ATOM	196	CD1	TYR	A	331	10.105	3.284	-24.334	1.00	34.66
	ATOM	197	CE1	TYR	A	331	9.985	2.228	-25.233	1.00	34.89
	ATOM	198	CD2	TYR	A	331	8.174	4.327	-25.287	1.00	37.88
20	ATOM	199	CE2	TYR	A	331	8.045	3.276	-26.193	1.00	34.65
	ATOM	200	CZ	TYR	A	331	8.950	2.232	-26.159	1.00	30.73
	ATOM	201	OH	TYR	A	331	8.814	1.191	-27.042	1.00	30.97
	ATOM	202	C	TYR	A	331	6.943	6.043	-22.754	1.00	46.24
	ATOM	203	O	TYR	A	331	6.018	5.301	-23.096	1.00	45.38
25	ATOM	204	N	ASP	A	332	6.868	7.372	-22.792	1.00	49.11
	ATOM	205	CA	ASP	A	332	5.684	8.092	-23.262	1.00	52.40
	ATOM	206	CB	ASP	A	332	5.781	8.321	-24.772	1.00	52.86
	ATOM	207	C	ASP	A	332	4.356	7.410	-22.926	1.00	52.90
	ATOM	208	O	ASP	A	332	3.561	7.116	-23.818	1.00	53.94
30	ATOM	209	N	PRO	A	333	4.103	7.144	-21.632	1.00	53.63
	ATOM	210	CD	PRO	A	333	4.962	7.418	-20.465	1.00	53.63
	ATOM	211	CA	PRO	A	333	2.840	6.497	-21.253	1.00	53.55
	ATOM	212	CB	PRO	A	333	3.070	6.076	-19.802	1.00	53.78
	ATOM	213	CG	PRO	A	333	4.101	7.028	-19.290	1.00	53.42
35	ATOM	214	C	PRO	A	333	1.673	7.478	-21.398	1.00	52.17
	ATOM	215	O	PRO	A	333	1.879	8.690	-21.395	1.00	51.19
	ATOM	216	N	THR	A	334	0.457	6.956	-21.532	1.00	52.26
	ATOM	217	CA	THR	A	334	-0.724	7.802	-21.687	1.00	54.21
	ATOM	218	CB	THR	A	334	-1.997	6.949	-21.813	1.00	53.90
40	ATOM	219	OG1	THR	A	334	-1.971	6.256	-23.065	1.00	53.92
	ATOM	220	CG2	THR	A	334	-3.237	7.821	-21.761	1.00	54.15
	ATOM	221	C	THR	A	334	-0.864	8.782	-20.525	1.00	56.34
	ATOM	222	O	THR	A	334	-1.389	8.443	-19.461	1.00	56.44
	ATOM	223	N	ARG	A	335	-0.386	10.002	-20.766	1.00	58.24
45	ATOM	224	CA	ARG	A	335	-0.377	11.099	-19.801	1.00	57.96
	ATOM	225	CB	ARG	A	335	-0.569	12.427	-20.531	1.00	60.22
	ATOM	226	C	ARG	A	335	-1.349	10.996	-18.627	1.00	56.61
	ATOM	227	O	ARG	A	335	-0.919	10.908	-17.475	1.00	60.70

ATOM	228	N	PRO	A	336	-2.667	11.015	-18.889	1.00	52.43
ATOM	229	CD	PRO	A	336	-3.389	11.117	-20.165	1.00	49.06
ATOM	230	CA	PRO	A	336	-3.587	10.915	-17.752	1.00	49.58
ATOM	231	CB	PRO	A	336	-4.911	11.456	-18.302	1.00	48.66
ATOM	232	CG	PRO	A	336	-4.645	11.809	-19.760	1.00	51.33
ATOM	233	C	PRO	A	336	-3.698	9.468	-17.279	1.00	49.25
ATOM	234	O	PRO	A	336	-4.340	8.644	-17.929	1.00	48.06
ATOM	235	N	PHE	A	337	-3.063	9.170	-16.147	1.00	47.90
ATOM	236	CA	PHE	A	337	-3.055	7.821	-15.582	1.00	46.61
ATOM	237	CB	PHE	A	337	-2.063	7.732	-14.421	1.00	47.73
ATOM	238	CG	PHE	A	337	-0.649	8.011	-14.805	1.00	46.27
ATOM	239	CD1	PHE	A	337	-0.017	9.168	-14.368	1.00	46.55
ATOM	240	CD2	PHE	A	337	0.061	7.113	-15.591	1.00	48.12
ATOM	241	CE1	PHE	A	337	1.305	9.429	-14.707	1.00	48.09
ATOM	242	CE2	PHE	A	337	1.386	7.364	-15.938	1.00	47.57
ATOM	243	CZ	PHE	A	337	2.009	8.525	-15.495	1.00	48.40
ATOM	244	C	PHE	A	337	-4.401	7.338	-15.071	1.00	46.15
ATOM	245	O	PHE	A	337	-5.250	8.127	-14.671	1.00	48.34
ATOM	246	N	SER	A	338	-4.573	6.022	-15.080	1.00	45.06
ATOM	247	CA	SER	A	338	-5.781	5.385	-14.578	1.00	45.12
ATOM	248	CB	SER	A	338	-6.477	4.594	-15.684	1.00	44.49
ATOM	249	OG	SER	A	338	-6.227	3.206	-15.554	1.00	45.78
ATOM	250	C	SER	A	338	-5.292	4.439	-13.488	1.00	47.04
ATOM	251	O	SER	A	338	-4.090	4.186	-13.387	1.00	44.08
ATOM	252	N	GLU	A	339	-6.206	3.916	-12.676	1.00	45.63
ATOM	253	CA	GLU	A	339	-5.802	3.012	-11.608	1.00	45.40
ATOM	254	CB	GLU	A	339	-7.015	2.521	-10.814	1.00	45.66
ATOM	255	CG	GLU	A	339	-6.637	1.680	-9.600	1.00	46.81
ATOM	256	CD	GLU	A	339	-7.717	1.652	-8.535	1.00	47.56
ATOM	257	OE1	GLU	A	339	-8.471	0.656	-8.477	1.00	47.37
ATOM	258	OE2	GLU	A	339	-7.810	2.625	-7.754	1.00	49.29
ATOM	259	C	GLU	A	339	-5.040	1.821	-12.170	1.00	45.23
ATOM	260	O	GLU	A	339	-3.862	1.641	-11.872	1.00	46.51
ATOM	261	N	ALA	A	340	-5.712	1.010	-12.982	1.00	42.87
ATOM	262	CA	ALA	A	340	-5.078	-0.158	-13.574	1.00	40.24
ATOM	263	CB	ALA	A	340	-6.055	-0.871	-14.496	1.00	41.40
ATOM	264	C	ALA	A	340	-3.837	0.273	-14.350	1.00	38.83
ATOM	265	O	ALA	A	340	-2.909	-0.515	-14.543	1.00	35.58
ATOM	266	N	SER	A	341	-3.836	1.535	-14.773	1.00	35.79
ATOM	267	CA	SER	A	341	-2.742	2.133	-15.537	1.00	36.58
ATOM	268	CB	SER	A	341	-3.231	3.454	-16.154	1.00	39.01
ATOM	269	OG	SER	A	341	-2.211	4.130	-16.864	1.00	36.09
ATOM	270	C	SER	A	341	-1.480	2.376	-14.691	1.00	35.63
ATOM	271	O	SER	A	341	-0.389	1.913	-15.038	1.00	33.20
ATOM	272	N	MET	A	342	-1.626	3.115	-13.595	1.00	35.92
ATOM	273	CA	MET	A	342	-0.498	3.396	-12.708	1.00	35.88
ATOM	274	CB	MET	A	342	-0.912	4.396	-11.623	1.00	35.96
ATOM	275	CG	MET	A	342	0.241	5.218	-11.059	1.00	38.02

ATOM	276	SD	MET	A	342	-0.308	6.374	-9.780	1.00	44.73
ATOM	277	CE	MET	A	342	0.626	7.815	-10.205	1.00	42.49
ATOM	278	C	MET	A	342	-0.011	2.100	-12.059	1.00	34.17
ATOM	279	O	MET	A	342	1.195	1.880	-11.909	1.00	33.40
ATOM	280	N	MET	A	343	-0.957	1.243	-11.687	1.00	29.95
ATOM	281	CA	MET	A	343	-0.640	-0.034	-11.062	1.00	31.96
ATOM	282	CB	MET	A	343	-1.921	-0.810	-10.751	1.00	31.70
ATOM	283	CG	MET	A	343	-2.667	-0.337	-9.502	1.00	37.13
ATOM	284	SD	MET	A	343	-1.749	-0.507	-7.940	1.00	36.00
ATOM	285	CE	MET	A	343	-1.468	-2.299	-7.886	1.00	32.14
ATOM	286	C	MET	A	343	0.234	-0.875	-11.979	1.00	31.72
ATOM	287	O	MET	A	343	1.159	-1.558	-11.527	1.00	30.26
ATOM	288	N	GLY	A	344	-0.069	-0.823	-13.272	1.00	29.04
ATOM	289	CA	GLY	A	344	0.688	-1.591	-14.242	1.00	24.94
ATOM	290	C	GLY	A	344	2.104	-1.085	-14.396	1.00	26.01
ATOM	291	O	GLY	A	344	3.046	-1.873	-14.463	1.00	28.72
ATOM	292	N	LEU	A	345	2.257	0.232	-14.471	1.00	26.97
ATOM	293	CA	LEU	A	345	3.576	0.839	-14.608	1.00	31.15
ATOM	294	CB	LEU	A	345	3.459	2.361	-14.753	1.00	30.06
ATOM	295	CG	LEU	A	345	2.765	2.924	-15.995	1.00	33.50
ATOM	296	CD1	LEU	A	345	2.901	4.439	-15.999	1.00	33.52
ATOM	297	CD2	LEU	A	345	3.379	2.324	-17.257	1.00	33.22
ATOM	298	C	LEU	A	345	4.433	0.534	-13.383	1.00	30.31
ATOM	299	O	LEU	A	345	5.564	0.061	-13.505	1.00	32.80
ATOM	300	N	LEU	A	346	3.884	0.813	-12.205	1.00	27.83
ATOM	301	CA	LEU	A	346	4.595	0.596	-10.947	1.00	26.19
ATOM	302	CB	LEU	A	346	3.729	1.063	-9.783	1.00	24.51
ATOM	303	CG	LEU	A	346	3.483	2.569	-9.682	1.00	26.33
ATOM	304	CD1	LEU	A	346	2.623	2.844	-8.463	1.00	27.33
ATOM	305	CD2	LEU	A	346	4.809	3.317	-9.587	1.00	24.89
ATOM	306	C	LEU	A	346	5.032	-0.848	-10.707	1.00	25.72
ATOM	307	O	LEU	A	346	6.181	-1.102	-10.345	1.00	29.86
ATOM	308	N	THR	A	347	4.117	-1.793	-10.891	1.00	23.80
ATOM	309	CA	THR	A	347	4.436	-3.196	-10.674	1.00	23.91
ATOM	310	CB	THR	A	347	3.164	-4.058	-10.641	1.00	26.39
ATOM	311	OG1	THR	A	347	2.421	-3.860	-11.849	1.00	24.57
ATOM	312	CG2	THR	A	347	2.301	-3.682	-9.444	1.00	23.98
ATOM	313	C	THR	A	347	5.366	-3.734	-11.756	1.00	26.17
ATOM	314	O	THR	A	347	6.176	-4.622	-11.496	1.00	27.44
ATOM	315	N	ASN	A	348	5.242	-3.197	-12.970	1.00	25.48
ATOM	316	CA	ASN	A	348	6.092	-3.617	-14.082	1.00	23.77
ATOM	317	CB	ASN	A	348	5.657	-2.926	-15.385	1.00	24.59
ATOM	318	CG	ASN	A	348	6.522	-3.302	-16.571	1.00	29.93
ATOM	319	OD1	ASN	A	348	7.616	-2.799	-16.771	1.00	24.81
ATOM	320	ND2	ASN	A	348	6.010	-4.236	-17.391	1.00	32.61
ATOM	321	C	ASN	A	348	7.532	-3.229	-13.741	1.00	22.82
ATOM	322	O	ASN	A	348	8.453	-4.027	-13.870	1.00	18.83
ATOM	323	N	LEU	A	349	7.711	-1.993	-13.288	1.00	22.58

ATOM	324	CA	LEU	A	349	9.030	-1.507	-12.914	1.00	21.85
ATOM	325	CB	LEU	A	349	8.929	-0.028	-12.536	1.00	22.00
ATOM	326	CG	LEU	A	349	10.155	0.673	-11.953	1.00	23.64
ATOM	327	CD1	LEU	A	349	11.224	0.826	-13.017	1.00	19.35
ATOM	328	CD2	LEU	A	349	9.726	2.040	-11.415	1.00	21.97
ATOM	329	C	LEU	A	349	9.564	-2.335	-11.734	1.00	22.94
ATOM	330	O	LEU	A	349	10.724	-2.749	-11.717	1.00	23.97
ATOM	331	N	ALA	A	350	8.705	-2.591	-10.756	1.00	21.67
ATOM	332	CA	ALA	A	350	9.113	-3.356	-9.586	1.00	21.83
ATOM	333	CB	ALA	A	350	7.963	-3.441	-8.593	1.00	18.95
ATOM	334	C	ALA	A	350	9.568	-4.757	-9.985	1.00	21.90
ATOM	335	O	ALA	A	350	10.625	-5.221	-9.554	1.00	24.15
ATOM	336	N	ASP	A	351	8.767	-5.423	-10.810	1.00	23.24
ATOM	337	CA	ASP	A	351	9.093	-6.772	-11.259	1.00	25.87
ATOM	338	CB	ASP	A	351	8.028	-7.274	-12.239	1.00	27.03
ATOM	339	CG	ASP	A	351	8.103	-8.772	-12.458	1.00	31.64
ATOM	340	OD1	ASP	A	351	8.217	-9.196	-13.628	1.00	35.06
ATOM	341	OD2	ASP	A	351	8.049	-9.525	-11.464	1.00	36.86
ATOM	342	C	ASP	A	351	10.469	-6.825	-11.912	1.00	22.36
ATOM	343	O	ASP	A	351	11.219	-7.773	-11.702	1.00	25.15
ATOM	344	N	ARG	A	352	10.810	-5.808	-12.697	1.00	23.58
ATOM	345	CA	ARG	A	352	12.115	-5.787	-13.347	1.00	21.07
ATOM	346	CB	ARG	A	352	12.120	-4.785	-14.507	1.00	21.02
ATOM	347	CG	ARG	A	352	11.539	-5.352	-15.797	1.00	20.44
ATOM	348	CD	ARG	A	352	11.554	-4.319	-16.915	1.00	20.43
ATOM	349	NE	ARG	A	352	10.592	-3.245	-16.687	1.00	19.85
ATOM	350	CZ	ARG	A	352	10.910	-1.954	-16.641	1.00	19.69
ATOM	351	NH1	ARG	A	352	12.172	-1.564	-16.813	1.00	17.36
ATOM	352	NH2	ARG	A	352	9.962	-1.049	-16.441	1.00	21.88
ATOM	353	C	ARG	A	352	13.223	-5.442	-12.350	1.00	22.11
ATOM	354	O	ARG	A	352	14.346	-5.945	-12.454	1.00	24.13
ATOM	355	N	GLU	A	353	12.909	-4.587	-11.383	1.00	18.66
ATOM	356	CA	GLU	A	353	13.888	-4.206	-10.376	1.00	19.08
ATOM	357	CB	GLU	A	353	13.317	-3.102	-9.483	1.00	21.62
ATOM	358	CG	GLU	A	353	13.295	-1.718	-10.114	1.00	20.97
ATOM	359	CD	GLU	A	353	12.832	-0.648	-9.129	1.00	23.84
ATOM	360	OE1	GLU	A	353	11.611	-0.531	-8.926	1.00	24.76
ATOM	361	OE2	GLU	A	353	13.686	0.066	-8.557	1.00	24.95
ATOM	362	C	GLU	A	353	14.246	-5.423	-9.512	1.00	20.14
ATOM	363	O	GLU	A	353	15.398	-5.600	-9.104	1.00	19.40
ATOM	364	N	LEU	A	354	13.246	-6.257	-9.235	1.00	19.54
ATOM	365	CA	LEU	A	354	13.434	-7.452	-8.415	1.00	21.77
ATOM	366	CB	LEU	A	354	12.107	-8.209	-8.270	1.00	23.09
ATOM	367	CG	LEU	A	354	11.160	-7.606	-7.223	1.00	25.00
ATOM	368	CD1	LEU	A	354	9.720	-8.013	-7.510	1.00	23.49
ATOM	369	CD2	LEU	A	354	11.584	-8.069	-5.839	1.00	23.31
ATOM	370	C	LEU	A	354	14.500	-8.386	-8.981	1.00	23.21
ATOM	371	O	LEU	A	354	15.255	-9.007	-8.234	1.00	22.44

	ATOM	372	N	VAL	A	355	14.560	-8.490	-10.302	1.00	22.52
	ATOM	373	CA	VAL	A	355	15.551	-9.343	-10.935	1.00	21.66
	ATOM	374	CB	VAL	A	355	15.353	-9.365	-12.466	1.00	24.35
	ATOM	375	CG1	VAL	A	355	16.435	-10.214	-13.119	1.00	28.16
5	ATOM	376	CG2	VAL	A	355	13.957	-9.886	-12.798	1.00	21.59
	ATOM	377	C	VAL	A	355	16.944	-8.811	-10.606	1.00	23.74
	ATOM	378	O	VAL	A	355	17.857	-9.581	-10.291	1.00	23.51
	ATOM	379	N	HIS	A	356	17.105	-7.489	-10.669	1.00	21.27
	ATOM	380	CA	HIS	A	356	18.392	-6.861	-10.369	1.00	21.31
10	ATOM	381	CB	HIS	A	356	18.384	-5.390	-10.811	1.00	19.87
	ATOM	382	CG	HIS	A	356	18.494	-5.205	-12.295	1.00	21.77
	ATOM	383	CD2	HIS	A	356	17.543	-5.048	-13.248	1.00	21.66
	ATOM	384	ND1	HIS	A	356	19.704	-5.177	-12.955	1.00	21.11
	ATOM	385	CE1	HIS	A	356	19.496	-5.011	-14.249	1.00	24.96
15	ATOM	386	NE2	HIS	A	356	18.192	-4.931	-14.455	1.00	18.37
	ATOM	387	C	HIS	A	356	18.702	-6.947	-8.875	1.00	21.41
	ATOM	388	O	HIS	A	356	19.864	-7.111	-8.465	1.00	21.88
	ATOM	389	N	MET	A	357	17.660	-6.843	-8.058	1.00	21.84
	ATOM	390	CA	MET	A	357	17.837	-6.906	-6.610	1.00	21.51
20	ATOM	391	CB	MET	A	357	16.503	-6.668	-5.898	1.00	17.60
	ATOM	392	CG	MET	A	357	16.629	-6.579	-4.369	1.00	19.36
	ATOM	393	SD	MET	A	357	15.051	-6.755	-3.531	1.00	23.64
	ATOM	394	CE	MET	A	357	14.189	-5.332	-4.163	1.00	23.13
	ATOM	395	C	MET	A	357	18.411	-8.259	-6.192	1.00	23.69
25	ATOM	396	O	MET	A	357	19.337	-8.328	-5.389	1.00	24.41
	ATOM	397	N	ILE	A	358	17.856	-9.331	-6.746	1.00	27.14
	ATOM	398	CA	ILE	A	358	18.314	-10.672	-6.425	1.00	28.79
	ATOM	399	CB	ILE	A	358	17.529	-11.725	-7.232	1.00	32.42
	ATOM	400	CG2	ILE	A	358	18.267	-13.064	-7.220	1.00	32.77
30	ATOM	401	CG1	ILE	A	358	16.125	-11.880	-6.644	1.00	31.94
	ATOM	402	CD1	ILE	A	358	15.062	-12.196	-7.680	1.00	34.85
	ATOM	403	C	ILE	A	358	19.801	-10.802	-6.728	1.00	28.75
	ATOM	404	O	ILE	A	358	20.569	-11.305	-5.912	1.00	31.60
	ATOM	405	N	ASN	A	359	20.207	-10.325	-7.897	1.00	27.91
35	ATOM	406	CA	ASN	A	359	21.601	-10.401	-8.293	1.00	29.16
	ATOM	407	CB	ASN	A	359	21.721	-10.172	-9.801	1.00	31.88
	ATOM	408	CG	ASN	A	359	21.253	-11.381	-10.599	1.00	39.34
	ATOM	409	OD1	ASN	A	359	21.916	-12.422	-10.612	1.00	41.27
	ATOM	410	ND2	ASN	A	359	20.102	-11.255	-11.253	1.00	38.58
40	ATOM	411	C	ASN	A	359	22.476	-9.436	-7.510	1.00	30.75
	ATOM	412	O	ASN	A	359	23.686	-9.629	-7.412	1.00	33.35
	ATOM	413	N	TRP	A	360	21.872	-8.400	-6.940	1.00	30.07
	ATOM	414	CA	TRP	A	360	22.634	-7.451	-6.132	1.00	27.87
	ATOM	415	CB	TRP	A	360	21.849	-6.150	-5.948	1.00	24.80
45	ATOM	416	CG	TRP	A	360	22.196	-5.392	-4.691	1.00	23.04
	ATOM	417	CD2	TRP	A	360	21.501	-5.443	-3.438	1.00	19.83
	ATOM	418	CE2	TRP	A	360	22.147	-4.543	-2.564	1.00	22.31
	ATOM	419	CE3	TRP	A	360	20.392	-6.165	-2.972	1.00	20.09

ATOM	420	CD1	TRP	A	360	23.212	-4.488	-4.529	1.00	18.99
ATOM	421	NE1	TRP	A	360	23.187	-3.974	-3.255	1.00	21.17
ATOM	422	CZ2	TRP	A	360	21.721	-4.340	-1.243	1.00	20.43
ATOM	423	CZ3	TRP	A	360	19.968	-5.965	-1.661	1.00	20.12
ATOM	424	CH2	TRP	A	360	20.635	-5.057	-0.812	1.00	18.54
ATOM	425	C	TRP	A	360	22.892	-8.099	-4.766	1.00	24.88
ATOM	426	O	TRP	A	360	23.978	-7.980	-4.198	1.00	25.00
ATOM	427	N	ALA	A	361	21.879	-8.789	-4.252	1.00	24.08
ATOM	428	CA	ALA	A	361	21.972	-9.462	-2.958	1.00	26.06
ATOM	429	CB	ALA	A	361	20.676	-10.203	-2.672	1.00	20.27
ATOM	430	C	ALA	A	361	23.161	-10.433	-2.897	1.00	28.44
ATOM	431	O	ALA	A	361	23.843	-10.531	-1.876	1.00	28.95
ATOM	432	N	LYS	A	362	23.414	-11.144	-3.992	1.00	31.41
ATOM	433	CA	LYS	A	362	24.530	-12.097	-4.047	1.00	33.33
ATOM	434	CB	LYS	A	362	24.564	-12.824	-5.390	1.00	34.81
ATOM	435	CG	LYS	A	362	23.319	-13.608	-5.756	1.00	36.27
ATOM	436	CD	LYS	A	362	23.458	-14.178	-7.167	1.00	38.30
ATOM	437	CE	LYS	A	362	22.369	-15.193	-7.472	1.00	40.94
ATOM	438	NZ	LYS	A	362	22.111	-15.322	-8.937	1.00	42.49
ATOM	439	C	LYS	A	362	25.854	-11.351	-3.893	1.00	34.17
ATOM	440	O	LYS	A	362	26.880	-11.977	-3.595	1.00	35.40
ATOM	441	N	AARG	A	363	25.826	-10.059	-4.095	0.50	34.23
ATOM	442	N	BARG	A	363	25.826	-10.059	-4.095	0.50	34.03
ATOM	443	CA	AARG	A	363	27.035	-9.254	-3.987	0.50	33.25
ATOM	444	CA	BARG	A	363	27.035	-9.254	-3.987	0.50	32.83
ATOM	445	CB	AARG	A	363	27.031	-8.153	-5.044	0.50	34.67
ATOM	446	CB	BARG	A	363	27.031	-8.153	-5.045	0.50	34.20
ATOM	447	CG	AARG	A	363	26.933	-8.654	-6.478	0.50	36.32
ATOM	448	CG	BARG	A	363	26.930	-8.654	-6.480	0.50	35.56
ATOM	449	CD	AARG	A	363	27.745	-7.775	-7.415	0.50	38.39
ATOM	450	CD	BARG	A	363	27.752	-7.781	-7.414	0.50	37.18
ATOM	451	NE	AARG	A	363	29.171	-7.793	-7.091	0.50	39.98
ATOM	452	NE	BARG	A	363	27.195	-7.725	-8.762	0.50	37.39
ATOM	453	CZ	AARG	A	363	30.086	-7.038	-7.692	0.50	40.54
ATOM	454	CZ	BARG	A	363	27.905	-7.457	-9.855	0.50	40.02
ATOM	455	NH1	AARG	A	363	29.735	-6.218	-8.675	0.50	38.13
ATOM	456	NH1	BARG	A	363	29.205	-7.191	-9.761	0.50	40.42
ATOM	457	NH2	AARG	A	363	31.358	-7.123	-7.326	0.50	43.19
ATOM	458	NH2	BARG	A	363	27.311	-7.436	-11.041	0.50	38.91
ATOM	459	C	AARG	A	363	27.207	-8.630	-2.610	0.50	33.28
ATOM	460	C	BARG	A	363	27.207	-8.630	-2.610	0.50	32.81
ATOM	461	O	AARG	A	363	28.223	-7.992	-2.344	0.50	34.18
ATOM	462	O	BARG	A	363	28.223	-7.992	-2.345	0.50	33.43
ATOM	463	N	VAL	A	364	26.215	-8.798	-1.740	1.00	33.12
ATOM	464	CA	VAL	A	364	26.288	-8.240	-0.389	1.00	33.63
ATOM	465	CB	VAL	A	364	24.898	-8.178	0.292	1.00	34.97
ATOM	466	CG1	VAL	A	364	25.036	-7.608	1.700	1.00	35.44
ATOM	467	CG2	VAL	A	364	23.946	-7.328	-0.532	1.00	36.69

	ATOM	468	C	VAL	A	364	27.184	-9.157	0.428	1.00	34.27
	ATOM	469	O	VAL	A	364	26.878	-10.341	0.603	1.00	34.95
	ATOM	470	N	PRO	A	365	28.306	-8.626	0.935	1.00	36.08
	ATOM	471	CD	PRO	A	365	28.775	-7.235	0.793	1.00	34.84
5	ATOM	472	CA	PRO	A	365	29.231	-9.442	1.733	1.00	37.82
	ATOM	473	CB	PRO	A	365	30.110	-8.408	2.430	1.00	34.31
	ATOM	474	CG	PRO	A	365	30.127	-7.247	1.475	1.00	37.77
	ATOM	475	C	PRO	A	365	28.538	-10.373	2.720	1.00	37.61
	ATOM	476	O	PRO	A	365	27.692	-9.945	3.507	1.00	37.74
10	ATOM	477	N	GLY	A	366	28.890	-11.654	2.654	1.00	39.04
	ATOM	478	CA	GLY	A	366	28.307	-12.635	3.554	1.00	38.27
	ATOM	479	C	GLY	A	366	26.991	-13.264	3.138	1.00	39.32
	ATOM	480	O	GLY	A	366	26.638	-14.336	3.635	1.00	39.53
	ATOM	481	N	PHE	A	367	26.246	-12.615	2.236	1.00	38.60
15	ATOM	482	CA	PHE	A	367	24.960	-13.148	1.783	1.00	36.36
	ATOM	483	CB	PHE	A	367	24.281	-12.178	0.808	1.00	32.10
	ATOM	484	CG	PHE	A	367	22.827	-12.473	0.581	1.00	30.12
	ATOM	485	CD1	PHE	A	367	22.401	-13.083	-0.596	1.00	28.95
	ATOM	486	CD2	PHE	A	367	21.882	-12.176	1.563	1.00	26.18
20	ATOM	487	CE1	PHE	A	367	21.050	-13.400	-0.792	1.00	29.42
	ATOM	488	CE2	PHE	A	367	20.535	-12.491	1.373	1.00	27.60
	ATOM	489	CZ	PHE	A	367	20.118	-13.103	0.196	1.00	26.81
	ATOM	490	C	PHE	A	367	25.072	-14.519	1.117	1.00	36.82
	ATOM	491	O	PHE	A	367	24.244	-15.398	1.359	1.00	36.55
25	ATOM	492	N	VAL	A	368	26.088	-14.694	0.276	1.00	38.28
	ATOM	493	CA	VAL	A	368	26.289	-15.965	-0.420	1.00	42.34
	ATOM	494	CB	VAL	A	368	27.386	-15.850	-1.504	1.00	41.78
	ATOM	495	CG1	VAL	A	368	26.972	-14.831	-2.550	1.00	44.60
	ATOM	496	CG2	VAL	A	368	28.707	-15.457	-0.873	1.00	42.23
30	ATOM	497	C	VAL	A	368	26.664	-17.100	0.533	1.00	43.85
	ATOM	498	O	VAL	A	368	26.469	-18.274	0.216	1.00	44.85
	ATOM	499	N	ASP	A	369	27.199	-16.750	1.699	1.00	44.93
	ATOM	500	CA	ASP	A	369	27.579	-17.755	2.688	1.00	44.96
	ATOM	501	CB	ASP	A	369	28.336	-17.106	3.849	1.00	43.76
35	ATOM	502	CG	ASP	A	369	29.608	-16.413	3.404	1.00	43.04
	ATOM	503	OD1	ASP	A	369	30.121	-15.570	4.167	1.00	44.32
	ATOM	504	OD2	ASP	A	369	30.097	-16.709	2.293	1.00	46.76
	ATOM	505	C	ASP	A	369	26.340	-18.465	3.228	1.00	45.89
	ATOM	506	O	ASP	A	369	26.360	-19.671	3.475	1.00	48.61
40	ATOM	507	N	LEU	A	370	25.261	-17.714	3.407	1.00	43.59
	ATOM	508	CA	LEU	A	370	24.020	-18.279	3.924	1.00	44.24
	ATOM	509	CB	LEU	A	370	22.980	-17.173	4.110	1.00	41.42
	ATOM	510	CG	LEU	A	370	23.404	-16.015	5.014	1.00	41.45
	ATOM	511	CD1	LEU	A	370	22.219	-15.095	5.245	1.00	42.25
45	ATOM	512	CD2	LEU	A	370	23.931	-16.552	6.332	1.00	38.35
	ATOM	513	C	LEU	A	370	23.449	-19.360	3.013	1.00	44.03
	ATOM	514	O	LEU	A	370	23.773	-19.423	1.829	1.00	43.63
	ATOM	515	N	THR	A	371	22.593	-20.206	3.575	1.00	44.29

ATOM	516	CA	THR	A	371	21.968	-21.272	2.806	1.00	44.84
ATOM	517	CB	THR	A	371	21.293	-22.302	3.730	1.00	45.65
ATOM	518	OG1	THR	A	371	20.262	-21.663	4.495	1.00	46.43
ATOM	519	CG2	THR	A	371	22.314	-22.903	4.677	1.00	46.48
ATOM	520	C	THR	A	371	20.923	-20.684	1.864	1.00	44.93
ATOM	521	O	THR	A	371	20.418	-19.585	2.092	1.00	44.36
ATOM	522	N	LEU	A	372	20.607	-21.418	0.804	1.00	43.83
ATOM	523	CA	LEU	A	372	19.624	-20.971	-0.166	1.00	44.62
ATOM	524	CB	LEU	A	372	19.407	-22.043	-1.237	1.00	47.17
ATOM	525	CG	LEU	A	372	18.512	-21.690	-2.429	1.00	46.91
ATOM	526	CD1	LEU	A	372	19.005	-20.417	-3.098	1.00	48.73
ATOM	527	CD2	LEU	A	372	18.521	-22.844	-3.420	1.00	51.12
ATOM	528	C	LEU	A	372	18.307	-20.644	0.512	1.00	44.84
ATOM	529	O	LEU	A	372	17.705	-19.602	0.261	1.00	43.25
ATOM	530	N	HIS	A	373	17.849	-21.558	1.382	1.00	43.14
ATOM	531	CA	HIS	A	373	16.599	-21.353	2.100	1.00	42.23
ATOM	532	CB	HIS	A	373	16.318	-22.525	3.062	1.00	45.38
ATOM	533	CG	HIS	A	373	15.114	-22.315	3.934	1.00	51.43
ATOM	534	CD2	HIS	A	373	13.808	-22.621	3.743	1.00	54.99
ATOM	535	ND1	HIS	A	373	15.187	-21.716	5.174	1.00	54.26
ATOM	536	CE1	HIS	A	373	13.979	-21.663	5.709	1.00	53.77
ATOM	537	NE2	HIS	A	373	13.124	-22.206	4.861	1.00	55.27
ATOM	538	C	HIS	A	373	16.665	-20.047	2.885	1.00	39.78
ATOM	539	O	HIS	A	373	15.677	-19.324	2.971	1.00	37.71
ATOM	540	N	ASP	A	374	17.839	-19.738	3.440	1.00	36.38
ATOM	541	CA	ASP	A	374	18.020	-18.516	4.219	1.00	37.21
ATOM	542	CB	ASP	A	374	19.287	-18.620	5.073	1.00	38.17
ATOM	543	CG	ASP	A	374	19.064	-19.425	6.344	1.00	41.47
ATOM	544	OD1	ASP	A	374	17.896	-19.543	6.772	1.00	37.09
ATOM	545	OD2	ASP	A	374	20.052	-19.940	6.912	1.00	44.40
ATOM	546	C	ASP	A	374	18.083	-17.277	3.326	1.00	37.19
ATOM	547	O	ASP	A	374	17.598	-16.208	3.696	1.00	38.13
ATOM	548	N	GLN	A	375	18.688	-17.431	2.152	1.00	33.13
ATOM	549	CA	GLN	A	375	18.788	-16.339	1.198	1.00	31.94
ATOM	550	CB	GLN	A	375	19.634	-16.756	-0.001	1.00	28.81
ATOM	551	CG	GLN	A	375	21.125	-16.570	0.189	1.00	31.71
ATOM	552	CD	GLN	A	375	21.920	-17.222	-0.922	1.00	34.49
ATOM	553	OE1	GLN	A	375	21.478	-17.267	-2.067	1.00	36.09
ATOM	554	NE2	GLN	A	375	23.097	-17.736	-0.588	1.00	40.32
ATOM	555	C	GLN	A	375	17.379	-16.009	0.730	1.00	31.50
ATOM	556	O	GLN	A	375	16.990	-14.840	0.653	1.00	27.42
ATOM	557	N	VAL	A	376	16.617	-17.056	0.429	1.00	30.38
ATOM	558	CA	VAL	A	376	15.242	-16.907	-0.027	1.00	33.50
ATOM	559	CB	VAL	A	376	14.588	-18.286	-0.286	1.00	30.57
ATOM	560	CG1	VAL	A	376	13.093	-18.122	-0.516	1.00	33.14
ATOM	561	CG2	VAL	A	376	15.232	-18.952	-1.485	1.00	30.79
ATOM	562	C	VAL	A	376	14.393	-16.159	1.002	1.00	33.80
ATOM	563	O	VAL	A	376	13.653	-15.237	0.661	1.00	34.89

	ATOM	564	N	HIS	A	377	14.500	-16.568	2.261	1.00	33.35
	ATOM	565	CA	HIS	A	377	13.730	-15.941	3.329	1.00	32.81
	ATOM	566	CB	HIS	A	377	13.966	-16.694	4.644	1.00	35.24
	ATOM	567	CG	HIS	A	377	13.429	-15.989	5.851	1.00	40.15
	ATOM	568	CD2	HIS	A	377	14.054	-15.495	6.946	1.00	40.86
	ATOM	569	ND1	HIS	A	377	12.090	-15.703	6.012	1.00	43.08
	ATOM	570	CE1	HIS	A	377	11.913	-15.062	7.154	1.00	42.44
	ATOM	571	NE2	HIS	A	377	13.089	-14.922	7.740	1.00	44.85
	ATOM	572	C	HIS	A	377	14.058	-14.454	3.507	1.00	28.63
	ATOM	573	O	HIS	A	377	13.158	-13.619	3.613	1.00	29.20
	ATOM	574	N	LEU	A	378	15.343	-14.125	3.544	1.00	24.41
	ATOM	575	CA	LEU	A	378	15.759	-12.738	3.721	1.00	23.21
	ATOM	576	CB	LEU	A	378	17.289	-12.650	3.743	1.00	20.98
	ATOM	577	CG	LEU	A	378	17.960	-13.190	5.016	1.00	24.22
	ATOM	578	CD1	LEU	A	378	19.471	-13.041	4.924	1.00	21.07
	ATOM	579	CD2	LEU	A	378	17.431	-12.446	6.221	1.00	20.24
	ATOM	580	C	LEU	A	378	15.190	-11.827	2.630	1.00	24.78
	ATOM	581	O	LEU	A	378	14.638	-10.766	2.922	1.00	22.09
	ATOM	582	N	LEU	A	379	15.321	-12.242	1.374	1.00	24.13
	ATOM	583	CA	LEU	A	379	14.812	-11.447	0.262	1.00	25.02
	ATOM	584	CB	LEU	A	379	15.307	-12.025	-1.062	1.00	27.12
	ATOM	585	CG	LEU	A	379	16.724	-11.600	-1.437	1.00	24.39
	ATOM	586	CD1	LEU	A	379	17.299	-12.557	-2.470	1.00	27.58
	ATOM	587	CD2	LEU	A	379	16.679	-10.178	-1.983	1.00	29.05
	ATOM	588	C	LEU	A	379	13.287	-11.355	0.246	1.00	27.61
	ATOM	589	O	LEU	A	379	12.726	-10.301	-0.062	1.00	26.16
	ATOM	590	N	GLU	A	380	12.616	-12.454	0.576	1.00	25.65
	ATOM	591	CA	GLU	A	380	11.154	-12.471	0.592	1.00	26.85
	ATOM	592	CB	GLU	A	380	10.640	-13.882	0.871	1.00	29.38
	ATOM	593	CG	GLU	A	380	10.718	-14.796	-0.331	1.00	35.58
	ATOM	594	CD	GLU	A	380	10.228	-16.194	-0.025	1.00	39.31
	ATOM	595	OE1	GLU	A	380	10.142	-17.008	-0.967	1.00	42.89
	ATOM	596	OE2	GLU	A	380	9.927	-16.478	1.153	1.00	39.45
	ATOM	597	C	GLU	A	380	10.604	-11.526	1.649	1.00	25.43
	ATOM	598	O	GLU	A	380	9.551	-10.925	1.469	1.00	27.75
	ATOM	599	N	CYS	A	381	11.324	-11.400	2.753	1.00	25.57
	ATOM	600	CA	CYS	A	381	10.907	-10.530	3.843	1.00	26.46
	ATOM	601	CB	CYS	A	381	11.570	-11.000	5.149	1.00	31.46
	ATOM	602	SG	CYS	A	381	11.305	-9.946	6.623	1.00	45.32
	ATOM	603	C	CYS	A	381	11.262	-9.059	3.589	1.00	24.77
	ATOM	604	O	CYS	A	381	10.516	-8.166	3.975	1.00	25.01
	ATOM	605	N	ALA	A	382	12.377	-8.815	2.903	1.00	22.23
	ATOM	606	CA	ALA	A	382	12.855	-7.449	2.681	1.00	21.83
	ATOM	607	CB	ALA	A	382	14.319	-7.383	3.095	1.00	21.56
	ATOM	608	C	ALA	A	382	12.705	-6.778	1.311	1.00	19.78
	ATOM	609	O	ALA	A	382	12.996	-5.587	1.182	1.00	17.01
	ATOM	610	N	TRP	A	383	12.261	-7.507	0.294	1.00	17.61
	ATOM	611	CA	TRP	A	383	12.164	-6.915	-1.036	1.00	18.06

	ATOM	612	CB	TRP	A	383	11.580	-7.928	-2.035	1.00	20.28
	ATOM	613	CG	TRP	A	383	10.105	-8.201	-1.919	1.00	20.50
	ATOM	614	CD2	TRP	A	383	9.049	-7.509	-2.599	1.00	22.48
	ATOM	615	CE2	TRP	A	383	7.836	-8.138	-2.238	1.00	20.41
5	ATOM	616	CE3	TRP	A	383	9.012	-6.420	-3.482	1.00	22.06
	ATOM	617	CD1	TRP	A	383	9.506	-9.189	-1.190	1.00	23.38
	ATOM	618	NE1	TRP	A	383	8.142	-9.159	-1.377	1.00	22.59
	ATOM	619	CZ2	TRP	A	383	6.598	-7.713	-2.724	1.00	21.98
	ATOM	620	CZ3	TRP	A	383	7.780	-5.998	-3.968	1.00	25.50
10	ATOM	621	CH2	TRP	A	383	6.589	-6.647	-3.587	1.00	23.11
	ATOM	622	C	TRP	A	383	11.448	-5.564	-1.170	1.00	19.18
	ATOM	623	O	TRP	A	383	11.972	-4.663	-1.824	1.00	19.27
	ATOM	624	N	LEU	A	384	10.273	-5.396	-0.567	1.00	18.32
	ATOM	625	CA	LEU	A	384	9.586	-4.118	-0.719	1.00	16.38
15	ATOM	626	CB	LEU	A	384	8.125	-4.218	-0.258	1.00	16.79
	ATOM	627	CG	LEU	A	384	7.211	-3.013	-0.577	1.00	18.39
	ATOM	628	CD1	LEU	A	384	7.464	-2.485	-1.995	1.00	13.91
	ATOM	629	CD2	LEU	A	384	5.750	-3.432	-0.410	1.00	18.38
	ATOM	630	C	LEU	A	384	10.324	-3.027	0.051	1.00	18.80
20	ATOM	631	O	LEU	A	384	10.334	-1.870	-0.357	1.00	20.90
	ATOM	632	N	GLU	A	385	10.949	-3.404	1.163	1.00	18.61
	ATOM	633	CA	GLU	A	385	11.718	-2.462	1.970	1.00	19.58
	ATOM	634	CB	GLU	A	385	12.274	-3.154	3.213	1.00	17.43
	ATOM	635	CG	GLU	A	385	11.292	-3.237	4.357	1.00	22.92
25	ATOM	636	CD	GLU	A	385	11.963	-3.676	5.640	1.00	25.83
	ATOM	637	OE1	GLU	A	385	12.431	-2.799	6.391	1.00	23.69
	ATOM	638	OE2	GLU	A	385	12.027	-4.897	5.889	1.00	27.64
	ATOM	639	C	GLU	A	385	12.890	-1.934	1.156	1.00	19.46
	ATOM	640	O	GLU	A	385	13.206	-0.743	1.196	1.00	15.04
30	ATOM	641	N	ILE	A	386	13.539	-2.842	0.431	1.00	13.32
	ATOM	642	CA	ILE	A	386	14.685	-2.484	-0.388	1.00	15.01
	ATOM	643	CB	ILE	A	386	15.475	-3.763	-0.807	1.00	17.43
	ATOM	644	CG2	ILE	A	386	16.544	-3.424	-1.849	1.00	17.99
	ATOM	645	CG1	ILE	A	386	16.185	-4.338	0.432	1.00	20.31
35	ATOM	646	CD1	ILE	A	386	16.682	-5.766	0.284	1.00	23.97
	ATOM	647	C	ILE	A	386	14.273	-1.645	-1.598	1.00	16.10
	ATOM	648	O	ILE	A	386	14.993	-0.724	-2.004	1.00	17.42
	ATOM	649	N	LEU	A	387	13.112	-1.944	-2.167	1.00	17.61
	ATOM	650	CA	LEU	A	387	12.620	-1.173	-3.304	1.00	18.20
40	ATOM	651	CB	LEU	A	387	11.359	-1.814	-3.882	1.00	17.51
	ATOM	652	CG	LEU	A	387	11.519	-3.064	-4.747	1.00	26.37
	ATOM	653	CD1	LEU	A	387	10.173	-3.406	-5.395	1.00	24.63
	ATOM	654	CD2	LEU	A	387	12.589	-2.824	-5.808	1.00	21.58
	ATOM	655	C	LEU	A	387	12.283	0.249	-2.838	1.00	17.60
45	ATOM	656	O	LEU	A	387	12.571	1.224	-3.530	1.00	17.15
	ATOM	657	N	MET	A	388	11.677	0.357	-1.660	1.00	17.65
	ATOM	658	CA	MET	A	388	11.286	1.656	-1.121	1.00	18.49
	ATOM	659	CB	MET	A	388	10.302	1.460	0.034	1.00	19.65

	ATOM	660	CG	MET	A	388	8.893	1.105	-0.435	1.00	15.12
	ATOM	661	SD	MET	A	388	7.744	0.769	0.910	1.00	18.73
	ATOM	662	CE	MET	A	388	6.163	0.908	0.048	1.00	18.34
	ATOM	663	C	MET	A	388	12.451	2.553	-0.691	1.00	22.62
5	ATOM	664	O	MET	A	388	12.417	3.767	-0.928	1.00	22.49
	ATOM	665	N	ILE	A	389	13.482	1.988	-0.064	1.00	21.45
	ATOM	666	CA	ILE	A	389	14.604	2.831	0.331	1.00	18.54
	ATOM	667	CB	ILE	A	389	15.590	2.108	1.299	1.00	19.35
	ATOM	668	CG2	ILE	A	389	16.362	0.998	0.578	1.00	15.50
10	ATOM	669	CG1	ILE	A	389	16.556	3.142	1.889	1.00	21.95
	ATOM	670	CD1	ILE	A	389	17.373	2.658	3.080	1.00	15.86
	ATOM	671	C	ILE	A	389	15.333	3.322	-0.922	1.00	18.67
	ATOM	672	O	ILE	A	389	15.813	4.453	-0.970	1.00	19.75
	ATOM	673	N	GLY	A	390	15.410	2.477	-1.943	1.00	20.58
15	ATOM	674	CA	GLY	A	390	16.049	2.895	-3.183	1.00	19.33
	ATOM	675	C	GLY	A	390	15.243	4.021	-3.819	1.00	17.48
	ATOM	676	O	GLY	A	390	15.801	4.994	-4.318	1.00	21.87
	ATOM	677	N	LEU	A	391	13.920	3.888	-3.787	1.00	19.17
	ATOM	678	CA	LEU	A	391	13.018	4.887	-4.343	1.00	21.50
20	ATOM	679	CB	LEU	A	391	11.561	4.420	-4.194	1.00	18.25
	ATOM	680	CG	LEU	A	391	10.480	5.497	-4.342	1.00	21.98
	ATOM	681	CD1	LEU	A	391	10.579	6.156	-5.725	1.00	21.39
	ATOM	682	CD2	LEU	A	391	9.115	4.868	-4.148	1.00	17.15
	ATOM	683	C	LEU	A	391	13.208	6.216	-3.620	1.00	23.27
25	ATOM	684	O	LEU	A	391	13.440	7.255	-4.243	1.00	23.60
	ATOM	685	N	VAL	A	392	13.122	6.170	-2.295	1.00	23.04
	ATOM	686	CA	VAL	A	392	13.282	7.357	-1.469	1.00	24.42
	ATOM	687	CB	VAL	A	392	13.186	6.993	0.042	1.00	27.38
	ATOM	688	CG1	VAL	A	392	13.733	8.129	0.897	1.00	30.37
30	ATOM	689	CG2	VAL	A	392	11.739	6.712	0.414	1.00	23.48
	ATOM	690	C	VAL	A	392	14.626	8.014	-1.754	1.00	27.55
	ATOM	691	O	VAL	A	392	14.728	9.242	-1.832	1.00	27.50
	ATOM	692	N	TRP	A	393	15.652	7.186	-1.924	1.00	23.65
	ATOM	693	CA	TRP	A	393	16.999	7.670	-2.204	1.00	24.76
35	ATOM	694	CB	TRP	A	393	17.977	6.491	-2.199	1.00	22.86
	ATOM	695	CG	TRP	A	393	19.287	6.784	-2.857	1.00	25.90
	ATOM	696	CD2	TRP	A	393	20.341	7.605	-2.339	1.00	28.09
	ATOM	697	CE2	TRP	A	393	21.375	7.612	-3.302	1.00	29.94
	ATOM	698	CE3	TRP	A	393	20.512	8.335	-1.154	1.00	30.20
40	ATOM	699	CD1	TRP	A	393	19.710	6.339	-4.077	1.00	26.55
	ATOM	700	NE1	TRP	A	393	20.963	6.833	-4.351	1.00	30.64
	ATOM	701	CZ2	TRP	A	393	22.566	8.323	-3.120	1.00	32.43
	ATOM	702	CZ3	TRP	A	393	21.698	9.044	-0.971	1.00	34.58
	ATOM	703	CH2	TRP	A	393	22.709	9.030	-1.950	1.00	36.54
45	ATOM	704	C	TRP	A	393	17.082	8.414	-3.547	1.00	25.02
	ATOM	705	O	TRP	A	393	17.767	9.435	-3.650	1.00	20.97
	ATOM	706	N	ARG	A	394	16.399	7.897	-4.568	1.00	23.06
	ATOM	707	CA	ARG	A	394	16.412	8.531	-5.890	1.00	25.97

	ATOM	708	CB	ARG	A	394	15.776	7.633	-6.965	1.00	24.05
	ATOM	709	CG	ARG	A	394	16.243	6.195	-7.024	1.00	26.05
	ATOM	710	CD	ARG	A	394	15.830	5.551	-8.352	1.00	22.70
	ATOM	711	NE	ARG	A	394	14.443	5.071	-8.363	1.00	20.71
5	ATOM	712	CZ	ARG	A	394	14.053	3.912	-7.841	1.00	21.26
	ATOM	713	NH1	ARG	A	394	14.944	3.108	-7.267	1.00	20.09
	ATOM	714	NH2	ARG	A	394	12.783	3.544	-7.907	1.00	21.26
	ATOM	715	C	ARG	A	394	15.622	9.833	-5.879	1.00	23.40
	ATOM	716	O	ARG	A	394	15.889	10.729	-6.677	1.00	28.61
10	ATOM	717	N	SER	A	395	14.638	9.924	-4.988	1.00	26.65
	ATOM	718	CA	SER	A	395	13.776	11.104	-4.902	1.00	27.46
	ATOM	719	CB	SER	A	395	12.395	10.696	-4.382	1.00	26.70
	ATOM	720	OG	SER	A	395	11.916	9.530	-5.029	1.00	22.95
	ATOM	721	C	SER	A	395	14.316	12.240	-4.033	1.00	31.45
15	ATOM	722	O	SER	A	395	13.726	13.324	-3.977	1.00	28.11
	ATOM	723	N	MET	A	396	15.437	11.986	-3.368	1.00	33.83
	ATOM	724	CA	MET	A	396	16.061	12.954	-2.475	1.00	38.83
	ATOM	725	CB	MET	A	396	17.466	12.483	-2.112	1.00	39.47
	ATOM	726	CG	MET	A	396	17.585	11.919	-0.715	1.00	41.37
20	ATOM	727	SD	MET	A	396	19.192	12.262	0.004	1.00	42.20
	ATOM	728	CE	MET	A	396	20.263	11.996	-1.404	1.00	42.84
	ATOM	729	C	MET	A	396	16.143	14.376	-3.018	1.00	40.69
	ATOM	730	O	MET	A	396	15.637	15.316	-2.403	1.00	38.85
	ATOM	731	N	GLU	A	397	16.794	14.526	-4.166	1.00	42.19
25	ATOM	732	CA	GLU	A	397	16.971	15.831	-4.790	1.00	44.80
	ATOM	733	CB	GLU	A	397	18.184	15.785	-5.729	1.00	46.02
	ATOM	734	CG	GLU	A	397	17.883	15.189	-7.096	1.00	54.42
	ATOM	735	CD	GLU	A	397	19.117	14.665	-7.810	1.00	59.40
	ATOM	736	OE1	GLU	A	397	19.219	13.430	-7.990	1.00	60.63
30	ATOM	737	OE2	GLU	A	397	19.980	15.485	-8.196	1.00	62.71
	ATOM	738	C	GLU	A	397	15.735	16.322	-5.554	1.00	42.94
	ATOM	739	O	GLU	A	397	15.830	17.229	-6.376	1.00	44.68
	ATOM	740	N	HIS	A	398	14.579	15.728	-5.280	1.00	40.82
	ATOM	741	CA	HIS	A	398	13.342	16.118	-5.950	1.00	39.21
35	ATOM	742	CB	HIS	A	398	12.924	15.043	-6.956	1.00	39.05
	ATOM	743	CG	HIS	A	398	13.870	14.886	-8.104	1.00	41.57
	ATOM	744	CD2	HIS	A	398	13.904	15.484	-9.318	1.00	39.28
	ATOM	745	ND1	HIS	A	398	14.940	14.017	-8.074	1.00	41.85
	ATOM	746	CE1	HIS	A	398	15.592	14.086	-9.220	1.00	40.88
40	ATOM	747	NE2	HIS	A	398	14.985	14.969	-9.993	1.00	42.30
	ATOM	748	C	HIS	A	398	12.216	16.332	-4.944	1.00	37.04
	ATOM	749	O	HIS	A	398	11.282	15.535	-4.864	1.00	36.51
	ATOM	750	N	PRO	A	399	12.283	17.427	-4.171	1.00	39.19
	ATOM	751	CD	PRO	A	399	13.328	18.467	-4.198	1.00	35.36
45	ATOM	752	CA	PRO	A	399	11.243	17.709	-3.173	1.00	37.10
	ATOM	753	CB	PRO	A	399	11.603	19.101	-2.654	1.00	37.86
	ATOM	754	CG	PRO	A	399	13.050	19.267	-2.963	1.00	35.83
	ATOM	755	C	PRO	A	399	9.828	17.663	-3.744	1.00	37.02

ATOM	756	O	PRO	A	399	9.554	18.249	-4.789	1.00	38.52
ATOM	757	N	GLY	A	400	8.938	16.954	-3.057	1.00	33.58
ATOM	758	CA	GLY	A	400	7.559	16.865	-3.503	1.00	32.12
ATOM	759	C	GLY	A	400	7.230	15.706	-4.428	1.00	32.43
ATOM	760	O	GLY	A	400	6.063	15.344	-4.574	1.00	33.21
ATOM	761	N	LYS	A	401	8.237	15.112	-5.055	1.00	31.35
ATOM	762	CA	LYS	A	401	7.972	14.007	-5.966	1.00	30.75
ATOM	763	CB	LYS	A	401	8.235	14.430	-7.415	1.00	35.43
ATOM	764	CG	LYS	A	401	8.130	15.927	-7.675	1.00	35.15
ATOM	765	CD	LYS	A	401	9.096	16.353	-8.774	1.00	36.88
ATOM	766	CE	LYS	A	401	8.733	17.721	-9.331	1.00	36.71
ATOM	767	NZ	LYS	A	401	7.295	18.027	-9.116	1.00	34.22
ATOM	768	C	LYS	A	401	8.768	12.746	-5.677	1.00	30.97
ATOM	769	O	LYS	A	401	9.809	12.776	-5.006	1.00	27.60
ATOM	770	N	LEU	A	402	8.256	11.635	-6.197	1.00	27.28
ATOM	771	CA	LEU	A	402	8.889	10.334	-6.050	1.00	29.07
ATOM	772	CB	LEU	A	402	7.866	9.294	-5.590	1.00	22.55
ATOM	773	CG	LEU	A	402	7.265	9.555	-4.207	1.00	24.94
ATOM	774	CD1	LEU	A	402	6.126	8.583	-3.937	1.00	19.32
ATOM	775	CD2	LEU	A	402	8.355	9.416	-3.157	1.00	21.54
ATOM	776	C	LEU	A	402	9.448	9.948	-7.414	1.00	28.78
ATOM	777	O	LEU	A	402	8.704	9.836	-8.389	1.00	29.98
ATOM	778	N	LEU	A	403	10.761	9.770	-7.487	1.00	27.57
ATOM	779	CA	LEU	A	403	11.393	9.400	-8.744	1.00	27.17
ATOM	780	CB	LEU	A	403	12.825	9.937	-8.816	1.00	26.95
ATOM	781	CG	LEU	A	403	13.401	10.027	-10.238	1.00	30.42
ATOM	782	CD1	LEU	A	403	14.519	11.046	-10.288	1.00	30.76
ATOM	783	CD2	LEU	A	403	13.915	8.665	-10.676	1.00	33.11
ATOM	784	C	LEU	A	403	11.419	7.891	-8.901	1.00	24.78
ATOM	785	O	LEU	A	403	12.428	7.257	-8.619	1.00	24.68
ATOM	786	N	PHE	A	404	10.306	7.319	-9.344	1.00	23.11
ATOM	787	CA	PHE	A	404	10.239	5.881	-9.546	1.00	26.93
ATOM	788	CB	PHE	A	404	8.826	5.470	-9.946	1.00	27.04
ATOM	789	CG	PHE	A	404	7.850	5.513	-8.816	1.00	27.89
ATOM	790	CD1	PHE	A	404	7.028	6.623	-8.631	1.00	26.20
ATOM	791	CD2	PHE	A	404	7.750	4.444	-7.925	1.00	23.10
ATOM	792	CE1	PHE	A	404	6.116	6.668	-7.573	1.00	25.29
ATOM	793	CE2	PHE	A	404	6.845	4.481	-6.870	1.00	21.01
ATOM	794	CZ	PHE	A	404	6.026	5.595	-6.693	1.00	22.91
ATOM	795	C	PHE	A	404	11.232	5.507	-10.637	1.00	26.04
ATOM	796	O	PHE	A	404	11.882	4.464	-10.578	1.00	27.27
ATOM	797	N	ALA	A	405	11.348	6.383	-11.626	1.00	28.80
ATOM	798	CA	ALA	A	405	12.271	6.195	-12.740	1.00	29.21
ATOM	799	CB	ALA	A	405	11.650	5.287	-13.806	1.00	26.89
ATOM	800	C	ALA	A	405	12.549	7.578	-13.317	1.00	30.23
ATOM	801	O	ALA	A	405	11.770	8.508	-13.109	1.00	27.38
ATOM	802	N	PRO	A	406	13.672	7.737	-14.032	1.00	30.05
ATOM	803	CD	PRO	A	406	14.712	6.745	-14.352	1.00	26.31

	ATOM	804	CA	PRO	A	406	13.977	9.053	-14.604	1.00	32.10
	ATOM	805	CB	PRO	A	406	15.232	8.800	-15.438	1.00	31.28
	ATOM	806	CG	PRO	A	406	15.865	7.602	-14.776	1.00	31.44
	ATOM	807	C	PRO	A	406	12.820	9.589	-15.436	1.00	32.58
5	ATOM	808	O	PRO	A	406	12.605	10.796	-15.507	1.00	32.58
	ATOM	809	N	ASN	A	407	12.063	8.690	-16.053	1.00	32.86
	ATOM	810	CA	ASN	A	407	10.935	9.119	-16.865	1.00	32.78
	ATOM	811	CB	ASN	A	407	10.950	8.418	-18.228	1.00	34.73
	ATOM	812	CG	ASN	A	407	10.884	6.907	-18.121	1.00	35.37
10	ATOM	813	OD1	ASN	A	407	11.189	6.317	-17.077	1.00	30.24
	ATOM	814	ND2	ASN	A	407	10.486	6.268	-19.215	1.00	34.08
	ATOM	815	C	ASN	A	407	9.605	8.901	-16.166	1.00	34.90
	ATOM	816	O	ASN	A	407	8.549	8.897	-16.798	1.00	36.09
	ATOM	817	N	LEU	A	408	9.660	8.724	-14.851	1.00	33.56
15	ATOM	818	CA	LEU	A	408	8.452	8.544	-14.061	1.00	35.59
	ATOM	819	CB	LEU	A	408	8.141	7.062	-13.851	1.00	33.81
	ATOM	820	CG	LEU	A	408	6.696	6.823	-13.397	1.00	36.44
	ATOM	821	CD1	LEU	A	408	5.746	7.479	-14.390	1.00	34.14
	ATOM	822	CD2	LEU	A	408	6.406	5.334	-13.287	1.00	32.96
20	ATOM	823	C	LEU	A	408	8.607	9.245	-12.717	1.00	38.03
	ATOM	824	O	LEU	A	408	8.880	8.614	-11.695	1.00	36.38
	ATOM	825	N	LEU	A	409	8.441	10.563	-12.741	1.00	37.87
	ATOM	826	CA	LEU	A	409	8.548	11.395	-11.553	1.00	37.95
	ATOM	827	CB	LEU	A	409	9.373	12.636	-11.877	1.00	39.52
25	ATOM	828	CG	LEU	A	409	10.023	13.399	-10.728	1.00	42.46
	ATOM	829	CD1	LEU	A	409	11.100	12.547	-10.082	1.00	43.24
	ATOM	830	CD2	LEU	A	409	10.614	14.691	-11.266	1.00	46.05
	ATOM	831	C	LEU	A	409	7.132	11.792	-11.163	1.00	37.13
	ATOM	832	O	LEU	A	409	6.482	12.546	-11.882	1.00	35.70
30	ATOM	833	N	LEU	A	410	6.654	11.284	-10.030	1.00	35.29
	ATOM	834	CA	LEU	A	410	5.297	11.576	-9.583	1.00	33.33
	ATOM	835	CB	LEU	A	410	4.503	10.277	-9.449	1.00	29.37
	ATOM	836	CG	LEU	A	410	4.645	9.238	-10.560	1.00	32.75
	ATOM	837	CD1	LEU	A	410	4.026	7.925	-10.104	1.00	29.16
35	ATOM	838	CD2	LEU	A	410	3.958	9.744	-11.819	1.00	30.70
	ATOM	839	C	LEU	A	410	5.207	12.332	-8.261	1.00	35.14
	ATOM	840	O	LEU	A	410	6.078	12.214	-7.400	1.00	36.94
	ATOM	841	N	ASP	A	411	4.141	13.108	-8.105	1.00	34.76
	ATOM	842	CA	ASP	A	411	3.933	13.843	-6.873	1.00	35.40
40	ATOM	843	CB	ASP	A	411	3.733	15.341	-7.144	1.00	40.02
	ATOM	844	CG	ASP	A	411	2.471	15.645	-7.928	1.00	41.32
	ATOM	845	OD1	ASP	A	411	1.570	14.785	-8.001	1.00	45.03
	ATOM	846	OD2	ASP	A	411	2.383	16.764	-8.474	1.00	45.01
	ATOM	847	C	ASP	A	411	2.727	13.234	-6.179	1.00	36.10
45	ATOM	848	O	ASP	A	411	2.033	12.395	-6.762	1.00	34.08
	ATOM	849	N	ARG	A	412	2.480	13.647	-4.940	1.00	35.99
	ATOM	850	CA	ARG	A	412	1.375	13.099	-4.169	1.00	39.37
	ATOM	851	CB	ARG	A	412	1.260	13.824	-2.825	1.00	39.75

	ATOM	852	CG	ARG	A	412	0.562	15.168	-2.870	1.00	40.49
	ATOM	853	CD	ARG	A	412	0.454	15.736	-1.465	1.00	40.65
	ATOM	854	NE	ARG	A	412	-0.261	14.826	-0.577	1.00	37.48
	ATOM	855	CZ	ARG	A	412	-1.574	14.855	-0.384	1.00	42.84
	ATOM	856	NH1	ARG	A	412	-2.316	15.754	-1.024	1.00	40.82
	ATOM	857	NH2	ARG	A	412	-2.150	13.986	0.438	1.00	38.32
	ATOM	858	C	ARG	A	412	0.034	13.108	-4.889	1.00	39.80
	ATOM	859	O	ARG	A	412	-0.775	12.201	-4.706	1.00	39.92
	ATOM	860	N	ASN	A	413	-0.198	14.119	-5.717	1.00	41.64
	ATOM	861	CA	ASN	A	413	-1.458	14.215	-6.440	1.00	43.19
	ATOM	862	CB	ASN	A	413	-1.518	15.533	-7.210	1.00	46.44
	ATOM	863	CG	ASN	A	413	-1.739	16.718	-6.299	1.00	47.86
	ATOM	864	OD1	ASN	A	413	-2.376	16.594	-5.249	1.00	48.05
	ATOM	865	ND2	ASN	A	413	-1.213	17.876	-6.687	1.00	49.43
	ATOM	866	C	ASN	A	413	-1.673	13.044	-7.385	1.00	41.48
	ATOM	867	O	ASN	A	413	-2.792	12.567	-7.546	1.00	40.50
	ATOM	868	N	GLN	A	414	-0.600	12.577	-8.010	1.00	42.82
	ATOM	869	CA	GLN	A	414	-0.703	11.448	-8.925	1.00	44.73
	ATOM	870	CB	GLN	A	414	0.585	11.307	-9.741	1.00	47.52
	ATOM	871	CG	GLN	A	414	0.572	12.088	-11.049	1.00	50.47
	ATOM	872	CD	GLN	A	414	1.914	12.713	-11.375	1.00	53.91
	ATOM	873	OE1	GLN	A	414	2.591	13.257	-10.501	1.00	53.68
	ATOM	874	NE2	GLN	A	414	2.309	12.637	-12.641	1.00	56.91
	ATOM	875	C	GLN	A	414	-0.970	10.163	-8.141	1.00	43.21
	ATOM	876	O	GLN	A	414	-1.491	9.193	-8.682	1.00	42.33
	ATOM	877	N	GLY	A	415	-0.618	10.168	-6.860	1.00	41.97
	ATOM	878	CA	GLY	A	415	-0.836	8.992	-6.040	1.00	40.43
	ATOM	879	C	GLY	A	415	-2.306	8.720	-5.804	1.00	40.80
	ATOM	880	O	GLY	A	415	-2.696	7.601	-5.472	1.00	37.83
	ATOM	881	N	LYS	A	416	-3.129	9.748	-5.978	1.00	42.16
	ATOM	882	CA	LYS	A	416	-4.566	9.613	-5.779	1.00	44.34
	ATOM	883	CB	LYS	A	416	-5.212	10.996	-5.704	1.00	45.65
	ATOM	884	CG	LYS	A	416	-4.761	11.819	-4.510	1.00	47.42
	ATOM	885	CD	LYS	A	416	-4.910	13.309	-4.777	1.00	50.97
	ATOM	886	CE	LYS	A	416	-5.992	13.924	-3.898	1.00	53.25
	ATOM	887	NZ	LYS	A	416	-5.416	14.764	-2.809	1.00	56.95
	ATOM	888	C	LYS	A	416	-5.227	8.793	-6.886	1.00	45.33
	ATOM	889	O	LYS	A	416	-6.339	8.299	-6.714	1.00	46.50
	ATOM	890	N	CYS	A	417	-4.540	8.648	-8.015	1.00	45.18
	ATOM	891	CA	CYS	A	417	-5.066	7.890	-9.148	1.00	46.25
	ATOM	892	CB	CYS	A	417	-4.062	7.902	-10.305	1.00	49.29
	ATOM	893	SG	CYS	A	417	-3.916	9.493	-11.168	1.00	49.59
	ATOM	894	C	CYS	A	417	-5.373	6.452	-8.752	1.00	47.18
	ATOM	895	O	CYS	A	417	-6.220	5.794	-9.359	1.00	46.50
	ATOM	896	N	VAL	A	418	-4.671	5.968	-7.731	1.00	45.07
	ATOM	897	CA	VAL	A	418	-4.866	4.612	-7.232	1.00	42.75
	ATOM	898	CB	VAL	A	418	-3.525	3.841	-7.206	1.00	42.45
	ATOM	899	CG1	VAL	A	418	-3.670	2.563	-6.410	1.00	40.22

ATOM	900	CG2	VAL	A	418	-3.071	3.538	-8.634	1.00	38.03
ATOM	901	C	VAL	A	418	-5.441	4.714	-5.818	1.00	41.46
ATOM	902	O	VAL	A	418	-4.883	5.400	-4.963	1.00	42.08
ATOM	903	N	GLU	A	419	-6.559	4.036	-5.579	1.00	40.95
ATOM	904	CA	GLU	A	419	-7.223	4.073	-4.275	1.00	42.51
ATOM	905	CB	GLU	A	419	-8.536	3.282	-4.333	1.00	44.52
ATOM	906	CG	GLU	A	419	-9.010	2.751	-2.984	1.00	50.42
ATOM	907	CD	GLU	A	419	-10.413	2.168	-3.035	1.00	54.38
ATOM	908	OE1	GLU	A	419	-10.582	1.059	-3.590	1.00	54.09
ATOM	909	OE2	GLU	A	419	-11.347	2.820	-2.516	1.00	57.90
ATOM	910	C	GLU	A	419	-6.370	3.552	-3.121	1.00	41.11
ATOM	911	O	GLU	A	419	-5.955	2.393	-3.116	1.00	39.42
ATOM	912	N	GLY	A	420	-6.129	4.419	-2.140	1.00	40.53
ATOM	913	CA	GLY	A	420	-5.346	4.049	-0.973	1.00	37.61
ATOM	914	C	GLY	A	420	-3.854	4.258	-1.140	1.00	37.01
ATOM	915	O	GLY	A	420	-3.088	4.105	-0.190	1.00	32.59
ATOM	916	N	MET	A	421	-3.444	4.623	-2.350	1.00	36.21
ATOM	917	CA	MET	A	421	-2.035	4.825	-2.656	1.00	36.02
ATOM	918	CB	MET	A	421	-1.799	4.607	-4.160	1.00	32.84
ATOM	919	CG	MET	A	421	-0.351	4.754	-4.617	1.00	35.82
ATOM	920	SD	MET	A	421	0.806	3.611	-3.812	1.00	35.57
ATOM	921	CE	MET	A	421	0.881	2.294	-5.005	1.00	32.51
ATOM	922	C	MET	A	421	-1.474	6.180	-2.226	1.00	34.93
ATOM	923	O	MET	A	421	-0.275	6.294	-1.985	1.00	35.17
ATOM	924	N	VAL	A	422	-2.319	7.205	-2.118	1.00	33.97
ATOM	925	CA	VAL	A	422	-1.823	8.520	-1.708	1.00	31.29
ATOM	926	CB	VAL	A	422	-2.927	9.607	-1.766	1.00	33.14
ATOM	927	CG1	VAL	A	422	-3.823	9.535	-0.533	1.00	30.10
ATOM	928	CG2	VAL	A	422	-2.279	10.982	-1.854	1.00	30.08
ATOM	929	C	VAL	A	422	-1.231	8.498	-0.296	1.00	32.64
ATOM	930	O	VAL	A	422	-0.274	9.220	0.002	1.00	28.41
ATOM	931	N	GLU	A	423	-1.803	7.670	0.571	1.00	31.53
ATOM	932	CA	GLU	A	423	-1.311	7.558	1.935	1.00	35.99
ATOM	933	CB	GLU	A	423	-2.190	6.594	2.737	1.00	40.37
ATOM	934	CG	GLU	A	423	-3.588	7.129	3.043	1.00	49.41
ATOM	935	CD	GLU	A	423	-4.438	7.336	1.795	1.00	52.38
ATOM	936	OE1	GLU	A	423	-5.349	8.188	1.835	1.00	56.91
ATOM	937	OE2	GLU	A	423	-4.200	6.652	0.776	1.00	54.53
ATOM	938	C	GLU	A	423	0.127	7.043	1.886	1.00	34.83
ATOM	939	O	GLU	A	423	1.007	7.552	2.581	1.00	31.85
ATOM	940	N	ILE	A	424	0.369	6.038	1.050	1.00	30.17
ATOM	941	CA	ILE	A	424	1.711	5.488	0.929	1.00	28.99
ATOM	942	CB	ILE	A	424	1.696	4.195	0.109	1.00	30.96
ATOM	943	CG2	ILE	A	424	3.108	3.588	0.068	1.00	27.20
ATOM	944	CG1	ILE	A	424	0.671	3.230	0.725	1.00	30.77
ATOM	945	CD1	ILE	A	424	0.810	1.787	0.291	1.00	34.69
ATOM	946	C	ILE	A	424	2.700	6.483	0.312	1.00	28.21
ATOM	947	O	ILE	A	424	3.856	6.551	0.735	1.00	28.48

ATOM	948	N	PHE	A	425	2.253	7.260	-0.675	1.00	27.68
ATOM	949	CA	PHE	A	425	3.119	8.253	-1.315	1.00	27.30
ATOM	950	CB	PHE	A	425	2.381	8.958	-2.458	1.00	26.36
ATOM	951	CG	PHE	A	425	2.538	8.289	-3.798	1.00	27.22
ATOM	952	CD1	PHE	A	425	2.619	9.050	-4.958	1.00	27.36
ATOM	953	CD2	PHE	A	425	2.566	6.900	-3.905	1.00	27.89
ATOM	954	CE1	PHE	A	425	2.721	8.443	-6.207	1.00	29.63
ATOM	955	CE2	PHE	A	425	2.668	6.282	-5.149	1.00	27.28
ATOM	956	CZ	PHE	A	425	2.745	7.056	-6.303	1.00	27.63
ATOM	957	C	PHE	A	425	3.591	9.306	-0.312	1.00	25.66
ATOM	958	O	PHE	A	425	4.757	9.713	-0.328	1.00	26.33
ATOM	959	N	ASP	A	426	2.680	9.746	0.552	1.00	27.92
ATOM	960	CA	ASP	A	426	2.984	10.759	1.570	1.00	28.88
ATOM	961	CB	ASP	A	426	1.721	11.102	2.369	1.00	32.58
ATOM	962	CG	ASP	A	426	0.781	12.034	1.613	1.00	37.47
ATOM	963	OD1	ASP	A	426	-0.432	12.039	1.925	1.00	37.72
ATOM	964	OD2	ASP	A	426	1.253	12.758	0.710	1.00	36.35
ATOM	965	C	ASP	A	426	4.071	10.278	2.532	1.00	26.96
ATOM	966	O	ASP	A	426	4.974	11.030	2.900	1.00	27.20
ATOM	967	N	MET	A	427	3.978	9.022	2.947	1.00	25.76
ATOM	968	CA	MET	A	427	4.981	8.468	3.856	1.00	25.89
ATOM	969	CB	MET	A	427	4.567	7.070	4.309	1.00	21.17
ATOM	970	CG	MET	A	427	3.385	7.072	5.257	1.00	24.38
ATOM	971	SD	MET	A	427	3.153	5.489	6.080	1.00	34.32
ATOM	972	CE	MET	A	427	2.173	4.637	4.910	1.00	21.03
ATOM	973	C	MET	A	427	6.321	8.410	3.128	1.00	22.29
ATOM	974	O	MET	A	427	7.363	8.760	3.689	1.00	22.19
ATOM	975	N	LEU	A	428	6.285	7.985	1.868	1.00	21.75
ATOM	976	CA	LEU	A	428	7.506	7.892	1.075	1.00	22.91
ATOM	977	CB	LEU	A	428	7.202	7.252	-0.287	1.00	18.47
ATOM	978	CG	LEU	A	428	6.910	5.747	-0.176	1.00	19.24
ATOM	979	CD1	LEU	A	428	6.278	5.222	-1.468	1.00	16.82
ATOM	980	CD2	LEU	A	428	8.204	5.010	0.131	1.00	16.23
ATOM	981	C	LEU	A	428	8.148	9.269	0.902	1.00	23.98
ATOM	982	O	LEU	A	428	9.366	9.416	1.034	1.00	23.06
ATOM	983	N	LEU	A	429	7.328	10.281	0.628	1.00	23.91
ATOM	984	CA	LEU	A	429	7.837	11.642	0.462	1.00	26.29
ATOM	985	CB	LEU	A	429	6.714	12.571	-0.003	1.00	27.47
ATOM	986	CG	LEU	A	429	6.331	12.411	-1.476	1.00	30.78
ATOM	987	CD1	LEU	A	429	5.022	13.139	-1.751	1.00	34.75
ATOM	988	CD2	LEU	A	429	7.449	12.952	-2.350	1.00	31.96
ATOM	989	C	LEU	A	429	8.425	12.166	1.776	1.00	25.83
ATOM	990	O	LEU	A	429	9.482	12.808	1.793	1.00	26.42
ATOM	991	N	ALA	A	430	7.734	11.890	2.877	1.00	26.45
ATOM	992	CA	ALA	A	430	8.201	12.333	4.185	1.00	26.11
ATOM	993	CB	ALA	A	430	7.214	11.909	5.265	1.00	23.13
ATOM	994	C	ALA	A	430	9.577	11.742	4.462	1.00	25.01
ATOM	995	O	ALA	A	430	10.455	12.409	5.005	1.00	24.31

ATOM	996	N	THR	A	431	9.767	10.486	4.074	1.00	25.25
ATOM	997	CA	THR	A	431	11.046	9.825	4.294	1.00	22.78
ATOM	998	CB	THR	A	431	10.973	8.323	3.962	1.00	21.36
ATOM	999	OG1	THR	A	431	9.924	7.727	4.727	1.00	20.27
ATOM	1000	CG2	THR	A	431	12.291	7.633	4.299	1.00	19.99
ATOM	1001	C	THR	A	431	12.103	10.477	3.429	1.00	23.73
ATOM	1002	O	THR	A	431	13.234	10.667	3.868	1.00	19.60
ATOM	1003	N	SER	A	432	11.736	10.819	2.197	1.00	24.32
ATOM	1004	CA	SER	A	432	12.676	11.479	1.301	1.00	26.96
ATOM	1005	CB	SER	A	432	12.067	11.650	-0.093	1.00	28.70
ATOM	1006	OG	SER	A	432	13.084	11.930	-1.039	1.00	33.42
ATOM	1007	C	SER	A	432	13.033	12.850	1.876	1.00	27.92
ATOM	1008	O	SER	A	432	14.176	13.294	1.779	1.00	30.78
ATOM	1009	N	SER	A	433	12.045	13.521	2.459	1.00	28.96
ATOM	1010	CA	SER	A	433	12.269	14.824	3.076	1.00	34.21
ATOM	1011	CB	SER	A	433	10.957	15.387	3.623	1.00	35.07
ATOM	1012	OG	SER	A	433	10.175	15.961	2.591	1.00	42.38
ATOM	1013	C	SER	A	433	13.263	14.644	4.223	1.00	33.43
ATOM	1014	O	SER	A	433	14.152	15.473	4.429	1.00	31.94
ATOM	1015	N	ARG	A	434	13.105	13.545	4.959	1.00	31.32
ATOM	1016	CA	ARG	A	434	13.980	13.236	6.086	1.00	29.78
ATOM	1017	CB	ARG	A	434	13.468	11.994	6.819	1.00	29.84
ATOM	1018	CG	ARG	A	434	14.331	11.541	7.983	1.00	32.17
ATOM	1019	CD	ARG	A	434	14.626	12.672	8.958	1.00	37.00
ATOM	1020	NE	ARG	A	434	15.321	12.169	10.140	1.00	39.44
ATOM	1021	CZ	ARG	A	434	15.935	12.935	11.034	1.00	44.06
ATOM	1022	NH1	ARG	A	434	15.949	14.255	10.885	1.00	45.52
ATOM	1023	NH2	ARG	A	434	16.528	12.381	12.084	1.00	45.01
ATOM	1024	C	ARG	A	434	15.413	13.014	5.605	1.00	29.24
ATOM	1025	O	ARG	A	434	16.352	13.563	6.173	1.00	29.72
ATOM	1026	N	PHE	A	435	15.577	12.206	4.561	1.00	28.95
ATOM	1027	CA	PHE	A	435	16.901	11.935	4.000	1.00	30.59
ATOM	1028	CB	PHE	A	435	16.777	11.045	2.758	1.00	32.03
ATOM	1029	CG	PHE	A	435	16.795	9.563	3.051	1.00	31.88
ATOM	1030	CD1	PHE	A	435	16.758	9.084	4.359	1.00	35.60
ATOM	1031	CD2	PHE	A	435	16.847	8.643	2.009	1.00	35.89
ATOM	1032	CE1	PHE	A	435	16.771	7.709	4.622	1.00	35.36
ATOM	1033	CE2	PHE	A	435	16.860	7.271	2.262	1.00	32.71
ATOM	1034	CZ	PHE	A	435	16.821	6.807	3.570	1.00	33.24
ATOM	1035	C	PHE	A	435	17.576	13.253	3.607	1.00	32.73
ATOM	1036	O	PHE	A	435	18.763	13.464	3.871	1.00	31.16
ATOM	1037	N	ARG	A	436	16.812	14.137	2.975	1.00	33.37
ATOM	1038	CA	ARG	A	436	17.341	15.429	2.549	1.00	39.13
ATOM	1039	CB	ARG	A	436	16.282	16.206	1.756	1.00	40.42
ATOM	1040	CG	ARG	A	436	16.846	17.317	0.877	1.00	43.09
ATOM	1041	CD	ARG	A	436	15.750	17.960	0.040	1.00	44.53
ATOM	1042	NE	ARG	A	436	14.826	16.955	-0.472	1.00	48.34
ATOM	1043	CZ	ARG	A	436	13.530	16.913	-0.184	1.00	48.81

	ATOM	1044	NH1	ARG	A	436	12.997	17.823	0.619	1.00	47.80
	ATOM	1045	NH2	ARG	A	436	12.769	15.950	-0.687	1.00	49.53
	ATOM	1046	C	ARG	A	436	17.792	16.250	3.753	1.00	38.10
	ATOM	1047	O	ARG	A	436	18.896	16.789	3.764	1.00	41.00
5	ATOM	1048	N	MET	A	437	16.936	16.334	4.766	1.00	39.47
	ATOM	1049	CA	MET	A	437	17.257	17.087	5.975	1.00	38.20
	ATOM	1050	CB	MET	A	437	16.102	16.998	6.965	1.00	39.79
	ATOM	1051	C	MET	A	437	18.550	16.594	6.626	1.00	41.15
	ATOM	1052	O	MET	A	437	19.303	17.378	7.201	1.00	40.20
10	ATOM	1053	N	MET	A	438	18.804	15.285	6.538	1.00	39.65
	ATOM	1054	CA	MET	A	438	20.011	14.693	7.117	1.00	39.70
	ATOM	1055	CB	MET	A	438	19.787	13.221	7.463	1.00	39.90
	ATOM	1056	CG	MET	A	438	18.694	12.938	8.460	1.00	41.94
	ATOM	1057	SD	MET	A	438	18.747	11.188	8.880	1.00	43.12
15	ATOM	1058	CE	MET	A	438	20.374	11.064	9.619	1.00	43.73
	ATOM	1059	C	MET	A	438	21.176	14.756	6.142	1.00	38.03
	ATOM	1060	O	MET	A	438	22.321	14.503	6.522	1.00	38.39
	ATOM	1061	N	ASN	A	439	20.886	15.070	4.895	1.00	37.64
	ATOM	1062	CA	ASN	A	439	21.924	15.118	3.895	1.00	35.68
20	ATOM	1063	CB	ASN	A	439	23.019	16.125	4.243	1.00	40.98
	ATOM	1064	CG	ASN	A	439	23.933	16.407	3.090	1.00	45.09
	ATOM	1065	OD1	ASN	A	439	23.528	16.295	1.934	1.00	47.16
	ATOM	1066	ND2	ASN	A	439	25.197	16.733	3.372	1.00	46.87
	ATOM	1067	C	ASN	A	439	22.552	13.732	3.739	1.00	31.06
25	ATOM	1068	O	ASN	A	439	23.764	13.581	3.649	1.00	29.54
	ATOM	1069	N	LEU	A	440	21.692	12.698	3.704	1.00	31.47
	ATOM	1070	CA	LEU	A	440	22.161	11.326	3.579	1.00	31.63
	ATOM	1071	CB	LEU	A	440	20.991	10.344	3.380	1.00	33.05
	ATOM	1072	CG	LEU	A	440	21.451	8.886	3.209	1.00	37.07
30	ATOM	1073	CD1	LEU	A	440	21.957	8.353	4.546	1.00	36.18
	ATOM	1074	CD2	LEU	A	440	20.318	8.032	2.682	1.00	32.33
	ATOM	1075	C	LEU	A	440	23.146	11.161	2.435	1.00	32.10
	ATOM	1076	O	LEU	A	440	22.925	11.671	1.333	1.00	32.76
	ATOM	1077	N	GLN	A	441	24.225	10.450	2.702	1.00	32.54
35	ATOM	1078	CA	GLN	A	441	25.255	10.220	1.699	1.00	31.97
	ATOM	1079	CB	GLN	A	441	26.632	10.320	2.345	1.00	31.75
	ATOM	1080	CG	GLN	A	441	26.896	11.669	2.979	1.00	35.56
	ATOM	1081	CD	GLN	A	441	27.040	12.748	1.939	1.00	34.97
	ATOM	1082	OE1	GLN	A	441	27.985	12.782	1.167	1.00	35.51
40	ATOM	1083	NE2	GLN	A	441	26.053	13.659	1.899	1.00	35.41
	ATOM	1084	C	GLN	A	441	25.100	8.860	1.038	1.00	34.08
	ATOM	1085	O	GLN	A	441	24.540	7.931	1.625	1.00	30.73
	ATOM	1086	N	GLY	A	442	25.608	8.752	-0.187	1.00	32.78
	ATOM	1087	CA	GLY	A	442	25.528	7.503	-0.921	1.00	32.91
45	ATOM	1088	C	GLY	A	442	26.181	6.350	-0.184	1.00	31.87
	ATOM	1089	O	GLY	A	442	25.642	5.245	-0.154	1.00	33.18
	ATOM	1090	N	GLU	A	443	27.340	6.603	0.416	1.00	30.60
	ATOM	1091	CA	GLU	A	443	28.057	5.567	1.150	1.00	30.85

	ATOM	1092	CB	GLU	A	443	29.376	6.111	1.704	1.00	32.74
	ATOM	1093	CG	GLU	A	443	30.425	6.378	0.646	1.00	36.30
	ATOM	1094	CD	GLU	A	443	30.310	7.770	0.066	1.00	40.92
	ATOM	1095	OE1	GLU	A	443	29.677	8.630	0.716	1.00	42.27
5	ATOM	1096	OE2	GLU	A	443	30.853	8.003	-1.038	1.00	46.82
	ATOM	1097	C	GLU	A	443	27.206	5.048	2.299	1.00	30.43
	ATOM	1098	O	GLU	A	443	27.211	3.854	2.595	1.00	28.11
	ATOM	1099	N	GLU	A	444	26.482	5.955	2.948	1.00	30.26
	ATOM	1100	CA	GLU	A	444	25.619	5.589	4.067	1.00	28.18
10	ATOM	1101	CB	GLU	A	444	25.147	6.843	4.797	1.00	26.32
	ATOM	1102	CG	GLU	A	444	26.250	7.633	5.463	1.00	29.27
	ATOM	1103	CD	GLU	A	444	25.748	8.944	6.023	1.00	29.62
	ATOM	1104	OE1	GLU	A	444	25.006	9.652	5.304	1.00	32.00
	ATOM	1105	OE2	GLU	A	444	26.088	9.268	7.182	1.00	29.02
15	ATOM	1106	C	GLU	A	444	24.403	4.813	3.572	1.00	26.93
	ATOM	1107	O	GLU	A	444	23.970	3.841	4.191	1.00	24.78
	ATOM	1108	N	PHE	A	445	23.861	5.256	2.443	1.00	27.79
	ATOM	1109	CA	PHE	A	445	22.688	4.633	1.853	1.00	24.50
	ATOM	1110	CB	PHE	A	445	22.254	5.416	0.610	1.00	25.40
20	ATOM	1111	CG	PHE	A	445	21.372	4.634	-0.316	1.00	23.74
	ATOM	1112	CD1	PHE	A	445	20.034	4.419	-0.004	1.00	23.00
	ATOM	1113	CD2	PHE	A	445	21.885	4.094	-1.489	1.00	22.37
	ATOM	1114	CE1	PHE	A	445	19.215	3.670	-0.855	1.00	22.57
	ATOM	1115	CE2	PHE	A	445	21.079	3.349	-2.342	1.00	21.69
25	ATOM	1116	CZ	PHE	A	445	19.741	3.138	-2.023	1.00	22.25
	ATOM	1117	C	PHE	A	445	22.913	3.169	1.489	1.00	22.81
	ATOM	1118	O	PHE	A	445	22.083	2.316	1.796	1.00	22.92
	ATOM	1119	N	VAL	A	446	24.019	2.868	0.822	1.00	22.46
	ATOM	1120	CA	VAL	A	446	24.278	1.481	0.447	1.00	22.26
30	ATOM	1121	CB	VAL	A	446	25.522	1.360	-0.465	1.00	22.87
	ATOM	1122	CG1	VAL	A	446	25.251	2.046	-1.799	1.00	22.57
	ATOM	1123	CG2	VAL	A	446	26.735	1.968	0.217	1.00	22.38
	ATOM	1124	C	VAL	A	446	24.467	0.614	1.694	1.00	23.68
	ATOM	1125	O	VAL	A	446	24.177	-0.586	1.680	1.00	22.91
35	ATOM	1126	N	CYS	A	447	24.962	1.223	2.770	1.00	22.02
	ATOM	1127	CA	CYS	A	447	25.155	0.503	4.025	1.00	24.17
	ATOM	1128	CB	CYS	A	447	25.953	1.359	5.011	1.00	23.95
	ATOM	1129	SG	CYS	A	447	27.738	1.324	4.731	1.00	28.57
	ATOM	1130	C	CYS	A	447	23.781	0.178	4.618	1.00	21.14
40	ATOM	1131	O	CYS	A	447	23.512	-0.960	5.002	1.00	19.37
	ATOM	1132	N	LEU	A	448	22.915	1.186	4.680	1.00	19.28
	ATOM	1133	CA	LEU	A	448	21.568	1.002	5.219	1.00	21.31
	ATOM	1134	CB	LEU	A	448	20.803	2.324	5.207	1.00	21.90
	ATOM	1135	CG	LEU	A	448	21.142	3.337	6.303	1.00	26.61
45	ATOM	1136	CD1	LEU	A	448	20.328	4.594	6.072	1.00	27.74
	ATOM	1137	CD2	LEU	A	448	20.827	2.760	7.672	1.00	24.03
	ATOM	1138	C	LEU	A	448	20.766	-0.038	4.442	1.00	21.72
	ATOM	1139	O	LEU	A	448	20.006	-0.803	5.030	1.00	20.87

	ATOM	1140	N	LYS	A	449	20.929	-0.055	3.119	1.00	21.42
	ATOM	1141	CA	LYS	A	449	20.205	-0.997	2.269	1.00	20.98
	ATOM	1142	CB	LYS	A	449	20.440	-0.659	0.788	1.00	21.55
	ATOM	1143	CG	LYS	A	449	19.438	-1.297	-0.173	1.00	24.82
5	ATOM	1144	CD	LYS	A	449	19.456	-0.613	-1.542	1.00	23.33
	ATOM	1145	CE	LYS	A	449	20.816	-0.754	-2.229	1.00	23.58
	ATOM	1146	NZ	LYS	A	449	20.741	-0.482	-3.698	1.00	28.77
	ATOM	1147	C	LYS	A	449	20.629	-2.436	2.548	1.00	20.33
	ATOM	1148	O	LYS	A	449	19.800	-3.345	2.552	1.00	20.57
10	ATOM	1149	N	SER	A	450	21.924	-2.637	2.777	1.00	19.25
	ATOM	1150	CA	SER	A	450	22.451	-3.965	3.074	1.00	21.84
	ATOM	1151	CB	SER	A	450	23.982	-3.953	3.041	1.00	20.59
	ATOM	1152	OG	SER	A	450	24.460	-3.975	1.702	1.00	29.78
	ATOM	1153	C	SER	A	450	21.975	-4.408	4.454	1.00	21.58
15	ATOM	1154	O	SER	A	450	21.728	-5.590	4.682	1.00	20.06
	ATOM	1155	N	ILE	A	451	21.853	-3.449	5.369	1.00	22.20
	ATOM	1156	CA	ILE	A	451	21.385	-3.741	6.726	1.00	22.82
	ATOM	1157	CB	ILE	A	451	21.452	-2.476	7.616	1.00	19.62
	ATOM	1158	CG2	ILE	A	451	20.593	-2.658	8.886	1.00	21.11
20	ATOM	1159	CG1	ILE	A	451	22.909	-2.210	7.999	1.00	22.20
	ATOM	1160	CD1	ILE	A	451	23.115	-0.960	8.850	1.00	24.48
	ATOM	1161	C	ILE	A	451	19.952	-4.250	6.662	1.00	21.82
	ATOM	1162	O	ILE	A	451	19.575	-5.184	7.369	1.00	21.72
	ATOM	1163	N	ILE	A	452	19.152	-3.642	5.795	1.00	20.18
25	ATOM	1164	CA	ILE	A	452	17.763	-4.058	5.649	1.00	18.13
	ATOM	1165	CB	ILE	A	452	17.024	-3.145	4.627	1.00	19.72
	ATOM	1166	CG2	ILE	A	452	15.720	-3.792	4.169	1.00	18.99
	ATOM	1167	CG1	ILE	A	452	16.725	-1.788	5.282	1.00	18.33
	ATOM	1168	CD1	ILE	A	452	16.284	-0.707	4.306	1.00	23.25
30	ATOM	1169	C	ILE	A	452	17.725	-5.517	5.191	1.00	19.50
	ATOM	1170	O	ILE	A	452	16.980	-6.340	5.737	1.00	17.60
	ATOM	1171	N	LEU	A	453	18.555	-5.844	4.209	1.00	19.23
	ATOM	1172	CA	LEU	A	453	18.589	-7.205	3.679	1.00	21.60
	ATOM	1173	CB	LEU	A	453	19.624	-7.316	2.554	1.00	21.50
35	ATOM	1174	CG	LEU	A	453	19.835	-8.729	1.989	1.00	25.06
	ATOM	1175	CD1	LEU	A	453	18.550	-9.250	1.364	1.00	25.27
	ATOM	1176	CD2	LEU	A	453	20.948	-8.694	0.953	1.00	24.73
	ATOM	1177	C	LEU	A	453	18.906	-8.245	4.746	1.00	19.41
	ATOM	1178	O	LEU	A	453	18.198	-9.241	4.891	1.00	20.75
40	ATOM	1179	N	LEU	A	454	19.966	-7.997	5.499	1.00	21.35
	ATOM	1180	CA	LEU	A	454	20.410	-8.925	6.530	1.00	23.67
	ATOM	1181	CB	LEU	A	454	21.870	-8.625	6.878	1.00	20.69
	ATOM	1182	CG	LEU	A	454	22.816	-8.584	5.673	1.00	24.92
	ATOM	1183	CD1	LEU	A	454	24.222	-8.268	6.132	1.00	24.27
45	ATOM	1184	CD2	LEU	A	454	22.785	-9.913	4.952	1.00	22.84
	ATOM	1185	C	LEU	A	454	19.572	-8.945	7.807	1.00	26.06
	ATOM	1186	O	LEU	A	454	19.413	-9.997	8.438	1.00	27.44
	ATOM	1187	N	ASN	A	455	19.011	-7.795	8.167	1.00	25.01

	ATOM	1188	CA	ASN	A	455	18.240	-7.681	9.400	1.00	26.10
	ATOM	1189	CB	ASN	A	455	18.439	-6.295	10.002	1.00	22.67
	ATOM	1190	CG	ASN	A	455	17.627	-6.109	11.264	1.00	26.67
	ATOM	1191	OD1	ASN	A	455	17.899	-6.751	12.270	1.00	25.16
5	ATOM	1192	ND2	ASN	A	455	16.615	-5.246	11.212	1.00	20.73
	ATOM	1193	C	ASN	A	455	16.739	-7.957	9.418	1.00	25.78
	ATOM	1194	O	ASN	A	455	16.230	-8.516	10.380	1.00	29.22
	ATOM	1195	N	SER	A	456	16.027	-7.549	8.381	1.00	28.51
	ATOM	1196	CA	SER	A	456	14.578	-7.704	8.371	1.00	32.52
10	ATOM	1197	CB	SER	A	456	14.019	-7.213	7.033	1.00	35.98
	ATOM	1198	OG	SER	A	456	14.266	-5.818	6.897	1.00	30.88
	ATOM	1199	C	SER	A	456	14.033	-9.086	8.711	1.00	33.00
	ATOM	1200	O	SER	A	456	13.112	-9.202	9.523	1.00	33.07
	ATOM	1201	N	GLY	A	457	14.597	-10.130	8.117	1.00	28.40
15	ATOM	1202	CA	GLY	A	457	14.115	-11.464	8.413	1.00	36.28
	ATOM	1203	C	GLY	A	457	15.055	-12.289	9.277	1.00	40.41
	ATOM	1204	O	GLY	A	457	14.831	-13.486	9.456	1.00	38.20
	ATOM	1205	N	VAL	A	458	16.095	-11.657	9.820	1.00	44.13
	ATOM	1206	CA	VAL	A	458	17.079	-12.356	10.647	1.00	51.09
20	ATOM	1207	CB	VAL	A	458	18.214	-11.399	11.095	1.00	51.06
	ATOM	1208	CG1	VAL	A	458	17.688	-10.390	12.104	1.00	51.75
	ATOM	1209	CG2	VAL	A	458	19.365	-12.199	11.692	1.00	50.65
	ATOM	1210	C	VAL	A	458	16.513	-13.060	11.885	1.00	57.26
	ATOM	1211	O	VAL	A	458	17.085	-14.045	12.356	1.00	58.77
25	ATOM	1212	N	TYR	A	459	15.401	-12.560	12.416	1.00	62.31
	ATOM	1213	CA	TYR	A	459	14.793	-13.177	13.592	1.00	68.49
	ATOM	1214	CB	TYR	A	459	14.293	-12.100	14.560	1.00	70.46
	ATOM	1215	CG	TYR	A	459	15.396	-11.196	15.069	1.00	71.73
	ATOM	1216	CD1	TYR	A	459	15.127	-9.888	15.462	1.00	71.93
30	ATOM	1217	CE1	TYR	A	459	16.147	-9.045	15.898	1.00	72.60
	ATOM	1218	CD2	TYR	A	459	16.716	-11.644	15.128	1.00	72.77
	ATOM	1219	CE2	TYR	A	459	17.741	-10.812	15.560	1.00	73.55
	ATOM	1220	CZ	TYR	A	459	17.450	-9.514	15.941	1.00	72.93
	ATOM	1221	OH	TYR	A	459	18.467	-8.687	16.351	1.00	74.56
35	ATOM	1222	C	TYR	A	459	13.649	-14.097	13.187	1.00	71.86
	ATOM	1223	O	TYR	A	459	13.380	-15.099	13.852	1.00	73.11
	ATOM	1224	N	THR	A	460	12.981	-13.756	12.090	1.00	74.84
	ATOM	1225	CA	THR	A	460	11.881	-14.567	11.589	1.00	77.66
	ATOM	1226	CB	THR	A	460	11.246	-13.900	10.373	1.00	76.69
40	ATOM	1227	C	THR	A	460	12.436	-15.938	11.212	1.00	80.26
	ATOM	1228	O	THR	A	460	11.684	-16.866	10.912	1.00	80.82
	ATOM	1229	N	PHE	A	461	13.762	-16.051	11.231	1.00	82.69
	ATOM	1230	CA	PHE	A	461	14.440	-17.299	10.905	1.00	85.63
	ATOM	1231	CB	PHE	A	461	15.920	-17.034	10.630	1.00	85.47
45	ATOM	1232	C	PHE	A	461	14.284	-18.288	12.059	1.00	87.52
	ATOM	1233	O	PHE	A	461	14.493	-17.940	13.224	1.00	86.53
	ATOM	1234	N	LEU	A	462	13.914	-19.520	11.724	1.00	89.49
	ATOM	1235	CA	LEU	A	462	13.711	-20.568	12.718	1.00	91.34

ATOM	1236	CB	LEU	A	462	12.961	-21.741	12.087	1.00	91.23
ATOM	1237	C	LEU	A	462	15.016	-21.060	13.340	1.00	92.05
ATOM	1238	O	LEU	A	462	16.042	-21.165	12.664	1.00	91.91
ATOM	1239	N	SER	A	463	14.966	-21.357	14.635	1.00	92.53
ATOM	1240	CA	SER	A	463	16.131	-21.855	15.358	1.00	92.96
ATOM	1241	CB	SER	A	463	16.033	-21.483	16.833	1.00	91.67
ATOM	1242	C	SER	A	463	16.189	-23.371	15.200	1.00	93.39
ATOM	1243	O	SER	A	463	15.156	-24.034	15.102	1.00	93.44
ATOM	1244	N	SER	A	464	17.399	-23.917	15.167	1.00	93.82
ATOM	1245	CA	SER	A	464	17.577	-25.355	15.015	1.00	93.85
ATOM	1246	CB	SER	A	464	17.284	-25.769	13.577	1.00	93.74
ATOM	1247	C	SER	A	464	18.997	-25.743	15.396	1.00	93.96
ATOM	1248	O	SER	A	464	19.815	-26.074	14.535	1.00	93.65
ATOM	1249	N	THR	A	465	19.279	-25.699	16.694	1.00	93.91
ATOM	1250	CA	THR	A	465	20.600	-26.036	17.212	1.00	93.79
ATOM	1251	CB	THR	A	465	20.952	-27.483	16.863	1.00	93.38
ATOM	1252	C	THR	A	465	21.640	-25.085	16.634	1.00	93.27
ATOM	1253	O	THR	A	465	21.302	-24.017	16.121	1.00	93.03
ATOM	1254	N	LEU	A	466	22.907	-25.479	16.723	1.00	93.26
ATOM	1255	CA	LEU	A	466	23.999	-24.665	16.207	1.00	92.34
ATOM	1256	CB	LEU	A	466	25.335	-25.338	16.498	1.00	91.59
ATOM	1257	C	LEU	A	466	23.829	-24.461	14.706	1.00	92.18
ATOM	1258	O	LEU	A	466	24.411	-23.545	14.125	1.00	92.67
ATOM	1259	N	LYS	A	467	23.028	-25.323	14.086	1.00	91.28
ATOM	1260	CA	LYS	A	467	22.772	-25.238	12.653	1.00	90.02
ATOM	1261	CB	LYS	A	467	21.740	-26.287	12.240	1.00	89.93
ATOM	1262	C	LYS	A	467	22.269	-23.841	12.308	1.00	88.35
ATOM	1263	O	LYS	A	467	23.032	-22.990	11.849	1.00	88.50
ATOM	1264	N	SER	A	468	20.981	-23.610	12.536	1.00	86.02
ATOM	1265	CA	SER	A	468	20.384	-22.315	12.252	1.00	84.10
ATOM	1266	CB	SER	A	468	18.901	-22.333	12.620	1.00	84.08
ATOM	1267	OG	SER	A	468	18.229	-23.378	11.937	1.00	83.03
ATOM	1268	C	SER	A	468	21.109	-21.230	13.040	1.00	83.39
ATOM	1269	O	SER	A	468	21.264	-20.105	12.565	1.00	83.48
ATOM	1270	N	LEU	A	469	21.558	-21.579	14.242	1.00	82.04
ATOM	1271	CA	LEU	A	469	22.276	-20.640	15.098	1.00	80.28
ATOM	1272	CB	LEU	A	469	22.595	-21.294	16.436	1.00	79.81
ATOM	1273	C	LEU	A	469	23.564	-20.174	14.419	1.00	79.18
ATOM	1274	O	LEU	A	469	24.111	-19.122	14.756	1.00	78.61
ATOM	1275	N	GLU	A	470	24.044	-20.969	13.466	1.00	76.69
ATOM	1276	CA	GLU	A	470	25.256	-20.638	12.726	1.00	74.84
ATOM	1277	CB	GLU	A	470	25.803	-21.880	12.032	1.00	74.12
ATOM	1278	C	GLU	A	470	24.920	-19.565	11.697	1.00	73.77
ATOM	1279	O	GLU	A	470	25.617	-18.556	11.581	1.00	72.94
ATOM	1280	N	GLU	A	471	23.842	-19.792	10.953	1.00	72.08
ATOM	1281	CA	GLU	A	471	23.396	-18.842	9.945	1.00	70.05
ATOM	1282	CB	GLU	A	471	22.461	-19.526	8.944	1.00	71.52
ATOM	1283	CG	GLU	A	471	23.150	-19.976	7.668	1.00	72.90

ATOM	1284	CD	GLU	A	471	24.512	-20.586	7.932	1.00	74.01
ATOM	1285	OE1	GLU	A	471	25.469	-20.258	7.198	1.00	74.22
ATOM	1286	OE2	GLU	A	471	24.626	-21.395	8.878	1.00	75.18
ATOM	1287	C	GLU	A	471	22.667	-17.692	10.630	1.00	67.33
ATOM	1288	O	GLU	A	471	21.685	-17.165	10.107	1.00	67.77
ATOM	1289	N	LYS	A	472	23.152	-17.319	11.811	1.00	62.63
ATOM	1290	CA	LYS	A	472	22.564	-16.229	12.578	1.00	57.41
ATOM	1291	CB	LYS	A	472	21.697	-16.777	13.713	1.00	58.74
ATOM	1292	CG	LYS	A	472	20.683	-15.776	14.243	1.00	60.32
ATOM	1293	CD	LYS	A	472	19.271	-16.342	14.219	1.00	60.73
ATOM	1294	CE	LYS	A	472	18.485	-15.909	15.449	1.00	61.78
ATOM	1295	NZ	LYS	A	472	19.352	-15.788	16.658	1.00	60.09
ATOM	1296	C	LYS	A	472	23.662	-15.339	13.150	1.00	53.42
ATOM	1297	O	LYS	A	472	23.631	-14.120	12.978	1.00	50.87
ATOM	1298	N	ASP	A	473	24.628	-15.949	13.830	1.00	47.52
ATOM	1299	CA	ASP	A	473	25.732	-15.194	14.405	1.00	45.55
ATOM	1300	CB	ASP	A	473	26.613	-16.094	15.269	1.00	50.48
ATOM	1301	CG	ASP	A	473	26.380	-15.885	16.749	1.00	55.50
ATOM	1302	OD1	ASP	A	473	25.272	-15.436	17.118	1.00	58.06
ATOM	1303	OD2	ASP	A	473	27.304	-16.170	17.541	1.00	59.81
ATOM	1304	C	ASP	A	473	26.557	-14.611	13.269	1.00	42.62
ATOM	1305	O	ASP	A	473	27.087	-13.506	13.373	1.00	42.10
ATOM	1306	N	HIS	A	474	26.663	-15.364	12.180	1.00	38.05
ATOM	1307	CA	HIS	A	474	27.416	-14.904	11.026	1.00	37.25
ATOM	1308	CB	HIS	A	474	27.429	-15.978	9.941	1.00	35.07
ATOM	1309	CG	HIS	A	474	28.036	-15.523	8.653	1.00	37.36
ATOM	1310	CD2	HIS	A	474	29.292	-15.113	8.355	1.00	38.86
ATOM	1311	ND1	HIS	A	474	27.322	-15.452	7.476	1.00	41.31
ATOM	1312	CE1	HIS	A	474	28.110	-15.020	6.509	1.00	40.86
ATOM	1313	NE2	HIS	A	474	29.311	-14.807	7.016	1.00	44.49
ATOM	1314	C	HIS	A	474	26.749	-13.640	10.493	1.00	36.68
ATOM	1315	O	HIS	A	474	27.417	-12.676	10.132	1.00	36.48
ATOM	1316	N	ILE	A	475	25.422	-13.652	10.447	1.00	35.93
ATOM	1317	CA	ILE	A	475	24.683	-12.499	9.963	1.00	36.21
ATOM	1318	CB	ILE	A	475	23.174	-12.797	9.868	1.00	36.31
ATOM	1319	CG2	ILE	A	475	22.411	-11.527	9.513	1.00	38.19
ATOM	1320	CG1	ILE	A	475	22.922	-13.874	8.813	1.00	36.97
ATOM	1321	CD1	ILE	A	475	21.528	-14.454	8.869	1.00	35.59
ATOM	1322	C	ILE	A	475	24.893	-11.322	10.907	1.00	35.34
ATOM	1323	O	ILE	A	475	25.092	-10.189	10.471	1.00	33.20
ATOM	1324	N	HIS	A	476	24.857	-11.596	12.206	1.00	35.95
ATOM	1325	CA	HIS	A	476	25.031	-10.540	13.193	1.00	35.06
ATOM	1326	CB	HIS	A	476	24.681	-11.062	14.585	1.00	37.30
ATOM	1327	CG	HIS	A	476	23.210	-11.068	14.860	1.00	43.06
ATOM	1328	CD2	HIS	A	476	22.329	-10.051	15.017	1.00	43.93
ATOM	1329	ND1	HIS	A	476	22.476	-12.230	14.968	1.00	45.60
ATOM	1330	CE1	HIS	A	476	21.207	-11.928	15.177	1.00	47.56
ATOM	1331	NE2	HIS	A	476	21.091	-10.613	15.211	1.00	46.21

ATOM	1332	C	HIS	A	476	26.438	-9.966	13.170	1.00	35.40
ATOM	1333	O	HIS	A	476	26.634	-8.774	13.415	1.00	35.45
ATOM	1334	N	ARG	A	477	27.420	-10.805	12.862	1.00	34.07
ATOM	1335	CA	ARG	A	477	28.796	-10.331	12.795	1.00	34.18
ATOM	1336	CB	ARG	A	477	29.757	-11.506	12.605	1.00	41.04
ATOM	1337	CG	ARG	A	477	29.800	-12.459	13.788	1.00	47.61
ATOM	1338	CD	ARG	A	477	30.782	-13.599	13.557	1.00	55.67
ATOM	1339	NE	ARG	A	477	31.780	-13.675	14.622	1.00	60.17
ATOM	1340	CZ	ARG	A	477	32.780	-12.811	14.770	1.00	61.98
ATOM	1341	NH1	ARG	A	477	32.918	-11.803	13.918	1.00	64.29
ATOM	1342	NH2	ARG	A	477	33.643	-12.955	15.766	1.00	62.79
ATOM	1343	C	ARG	A	477	28.906	-9.361	11.621	1.00	30.77
ATOM	1344	O	ARG	A	477	29.462	-8.268	11.753	1.00	33.59
ATOM	1345	N	VAL	A	478	28.369	-9.766	10.475	1.00	27.65
ATOM	1346	CA	VAL	A	478	28.389	-8.930	9.280	1.00	27.07
ATOM	1347	CB	VAL	A	478	27.658	-9.605	8.100	1.00	28.00
ATOM	1348	CG1	VAL	A	478	27.672	-8.678	6.890	1.00	25.83
ATOM	1349	CG2	VAL	A	478	28.319	-10.933	7.761	1.00	31.66
ATOM	1350	C	VAL	A	478	27.689	-7.610	9.584	1.00	26.92
ATOM	1351	O	VAL	A	478	28.216	-6.536	9.294	1.00	26.97
ATOM	1352	N	LEU	A	479	26.499	-7.702	10.171	1.00	25.74
ATOM	1353	CA	LEU	A	479	25.727	-6.516	10.530	1.00	27.97
ATOM	1354	CB	LEU	A	479	24.474	-6.912	11.324	1.00	25.55
ATOM	1355	CG	LEU	A	479	23.211	-7.229	10.517	1.00	29.01
ATOM	1356	CD1	LEU	A	479	22.056	-7.503	11.481	1.00	27.05
ATOM	1357	CD2	LEU	A	479	22.864	-6.063	9.584	1.00	24.92
ATOM	1358	C	LEU	A	479	26.592	-5.582	11.369	1.00	25.39
ATOM	1359	O	LEU	A	479	26.595	-4.370	11.158	1.00	27.39
ATOM	1360	N	ASP	A	480	27.324	-6.158	12.320	1.00	26.04
ATOM	1361	CA	ASP	A	480	28.206	-5.388	13.193	1.00	27.32
ATOM	1362	CB	ASP	A	480	28.878	-6.305	14.222	1.00	26.67
ATOM	1363	CG	ASP	A	480	27.990	-6.602	15.417	1.00	31.02
ATOM	1364	OD1	ASP	A	480	28.355	-7.505	16.198	1.00	31.50
ATOM	1365	OD2	ASP	A	480	26.935	-5.944	15.580	1.00	32.21
ATOM	1366	C	ASP	A	480	29.283	-4.699	12.361	1.00	25.59
ATOM	1367	O	ASP	A	480	29.672	-3.562	12.636	1.00	27.15
ATOM	1368	N	LYS	A	481	29.767	-5.394	11.340	1.00	25.17
ATOM	1369	CA	LYS	A	481	30.794	-4.830	10.477	1.00	24.93
ATOM	1370	CB	LYS	A	481	31.306	-5.890	9.512	1.00	28.42
ATOM	1371	CG	LYS	A	481	32.158	-6.953	10.188	1.00	35.59
ATOM	1372	CD	LYS	A	481	32.894	-7.799	9.157	1.00	41.21
ATOM	1373	CE	LYS	A	481	33.883	-6.963	8.350	1.00	41.48
ATOM	1374	NZ	LYS	A	481	34.954	-6.388	9.215	1.00	43.22
ATOM	1375	C	LYS	A	481	30.260	-3.635	9.696	1.00	26.12
ATOM	1376	O	LYS	A	481	30.979	-2.657	9.463	1.00	23.73
ATOM	1377	N	ILE	A	482	28.996	-3.705	9.291	1.00	25.44
ATOM	1378	CA	ILE	A	482	28.421	-2.598	8.545	1.00	27.69
ATOM	1379	CB	ILE	A	482	27.066	-2.983	7.915	1.00	27.59

ATOM	1380	CG2	ILE	A	482	26.470	-1.788	7.183	1.00	25.97
ATOM	1381	CG1	ILE	A	482	27.274	-4.131	6.922	1.00	23.80
ATOM	1382	CD1	ILE	A	482	26.000	-4.838	6.533	1.00	21.30
ATOM	1383	C	ILE	A	482	28.253	-1.408	9.481	1.00	27.33
ATOM	1384	O	ILE	A	482	28.312	-0.256	9.045	1.00	28.55
ATOM	1385	N	THR	A	483	28.046	-1.690	10.768	1.00	25.03
ATOM	1386	CA	THR	A	483	27.905	-0.632	11.760	1.00	23.62
ATOM	1387	CB	THR	A	483	27.535	-1.192	13.154	1.00	22.18
ATOM	1388	OG1	THR	A	483	26.181	-1.658	13.133	1.00	25.39
ATOM	1389	CG2	THR	A	483	27.673	-0.111	14.226	1.00	25.84
ATOM	1390	C	THR	A	483	29.257	0.074	11.858	1.00	23.04
ATOM	1391	O	THR	A	483	29.331	1.306	11.846	1.00	23.55
ATOM	1392	N	ASP	A	484	30.324	-0.714	11.960	1.00	22.24
ATOM	1393	CA	ASP	A	484	31.674	-0.152	12.039	1.00	25.48
ATOM	1394	CB	ASP	A	484	32.718	-1.273	12.107	1.00	26.88
ATOM	1395	CG	ASP	A	484	32.629	-2.083	13.394	1.00	32.52
ATOM	1396	OD1	ASP	A	484	32.002	-1.608	14.366	1.00	33.68
ATOM	1397	OD2	ASP	A	484	33.185	-3.198	13.434	1.00	34.63
ATOM	1398	C	ASP	A	484	31.930	0.715	10.807	1.00	25.16
ATOM	1399	O	ASP	A	484	32.481	1.812	10.905	1.00	26.05
ATOM	1400	N	THR	A	485	31.505	0.226	9.645	1.00	28.96
ATOM	1401	CA	THR	A	485	31.689	0.960	8.394	1.00	26.63
ATOM	1402	CB	THR	A	485	31.124	0.166	7.197	1.00	26.12
ATOM	1403	OG1	THR	A	485	31.753	-1.123	7.132	1.00	24.30
ATOM	1404	CG2	THR	A	485	31.381	0.907	5.898	1.00	23.31
ATOM	1405	C	THR	A	485	30.994	2.318	8.468	1.00	28.90
ATOM	1406	O	THR	A	485	31.583	3.354	8.137	1.00	27.26
ATOM	1407	N	LEU	A	486	29.743	2.310	8.915	1.00	24.76
ATOM	1408	CA	LEU	A	486	28.973	3.537	9.027	1.00	26.19
ATOM	1409	CB	LEU	A	486	27.567	3.233	9.547	1.00	27.27
ATOM	1410	CG	LEU	A	486	26.508	2.921	8.486	1.00	23.50
ATOM	1411	CD1	LEU	A	486	25.210	2.550	9.183	1.00	22.03
ATOM	1412	CD2	LEU	A	486	26.309	4.128	7.577	1.00	21.35
ATOM	1413	C	LEU	A	486	29.662	4.519	9.960	1.00	27.36
ATOM	1414	O	LEU	A	486	29.745	5.710	9.669	1.00	25.87
ATOM	1415	N	ILE	A	487	30.151	4.015	11.088	1.00	27.88
ATOM	1416	CA	ILE	A	487	30.843	4.857	12.055	1.00	28.40
ATOM	1417	CB	ILE	A	487	31.203	4.054	13.332	1.00	26.74
ATOM	1418	CG2	ILE	A	487	32.255	4.803	14.154	1.00	27.54
ATOM	1419	CG1	ILE	A	487	29.937	3.813	14.163	1.00	25.93
ATOM	1420	CD1	ILE	A	487	29.237	5.088	14.624	1.00	23.42
ATOM	1421	C	ILE	A	487	32.125	5.393	11.412	1.00	28.89
ATOM	1422	O	ILE	A	487	32.497	6.554	11.602	1.00	29.85
ATOM	1423	N	HIS	A	488	32.791	4.533	10.649	1.00	29.71
ATOM	1424	CA	HIS	A	488	34.031	4.898	9.967	1.00	34.12
ATOM	1425	CB	HIS	A	488	34.585	3.691	9.207	1.00	36.61
ATOM	1426	CG	HIS	A	488	35.799	3.997	8.385	1.00	42.74
ATOM	1427	CD2	HIS	A	488	35.970	4.089	7.045	1.00	43.12

ATOM	1428	ND1	HIS	A	488	37.034	4.239	8.946	1.00	43.13
ATOM	1429	CE1	HIS	A	488	37.913	4.466	7.987	1.00	43.40
ATOM	1430	NE2	HIS	A	488	37.293	4.381	6.825	1.00	45.63
ATOM	1431	C	HIS	A	488	33.799	6.051	8.998	1.00	32.74
ATOM	1432	O	HIS	A	488	34.577	7.004	8.955	1.00	31.06
ATOM	1433	N	LEU	A	489	32.721	5.958	8.223	1.00	33.56
ATOM	1434	CA	LEU	A	489	32.384	6.992	7.258	1.00	30.78
ATOM	1435	CB	LEU	A	489	31.145	6.587	6.464	1.00	34.67
ATOM	1436	CG	LEU	A	489	31.310	5.353	5.574	1.00	34.73
ATOM	1437	CD1	LEU	A	489	29.945	4.856	5.125	1.00	33.21
ATOM	1438	CD2	LEU	A	489	32.183	5.701	4.378	1.00	35.92
ATOM	1439	C	LEU	A	489	32.124	8.320	7.954	1.00	33.97
ATOM	1440	O	LEU	A	489	32.587	9.365	7.507	1.00	33.22
ATOM	1441	N	MET	A	490	31.387	8.274	9.058	1.00	31.33
ATOM	1442	CA	MET	A	490	31.056	9.482	9.801	1.00	30.61
ATOM	1443	CB	MET	A	490	30.000	9.161	10.862	1.00	32.34
ATOM	1444	CG	MET	A	490	28.607	8.940	10.289	1.00	30.71
ATOM	1445	SD	MET	A	490	27.457	8.247	11.496	1.00	31.14
ATOM	1446	CE	MET	A	490	26.321	7.408	10.418	1.00	30.36
ATOM	1447	C	MET	A	490	32.287	10.108	10.455	1.00	32.22
ATOM	1448	O	MET	A	490	32.412	11.330	10.517	1.00	28.25
ATOM	1449	N	ALA	A	491	33.184	9.262	10.949	1.00	33.81
ATOM	1450	CA	ALA	A	491	34.407	9.730	11.585	1.00	39.92
ATOM	1451	CB	ALA	A	491	35.168	8.554	12.185	1.00	37.22
ATOM	1452	C	ALA	A	491	35.275	10.445	10.550	1.00	42.68
ATOM	1453	O	ALA	A	491	35.865	11.487	10.838	1.00	45.32
ATOM	1454	N	LYS	A	492	35.339	9.876	9.347	1.00	44.39
ATOM	1455	CA	LYS	A	492	36.122	10.440	8.248	1.00	44.80
ATOM	1456	CB	LYS	A	492	36.136	9.477	7.052	1.00	46.96
ATOM	1457	CG	LYS	A	492	37.490	8.840	6.744	1.00	47.20
ATOM	1458	CD	LYS	A	492	37.390	7.830	5.595	1.00	45.71
ATOM	1459	CE	LYS	A	492	38.631	6.937	5.518	1.00	45.55
ATOM	1460	NZ	LYS	A	492	38.357	5.577	4.948	1.00	36.28
ATOM	1461	C	LYS	A	492	35.534	11.780	7.809	1.00	45.61
ATOM	1462	O	LYS	A	492	36.227	12.604	7.215	1.00	46.18
ATOM	1463	N	ALA	A	493	34.254	11.992	8.100	1.00	43.75
ATOM	1464	CA	ALA	A	493	33.590	13.238	7.728	1.00	42.42
ATOM	1465	CB	ALA	A	493	32.097	13.001	7.528	1.00	40.92
ATOM	1466	C	ALA	A	493	33.816	14.305	8.796	1.00	41.78
ATOM	1467	O	ALA	A	493	33.277	15.410	8.707	1.00	40.76
ATOM	1468	N	GLY	A	494	34.604	13.960	9.811	1.00	41.01
ATOM	1469	CA	GLY	A	494	34.903	14.904	10.873	1.00	41.63
ATOM	1470	C	GLY	A	494	33.857	15.060	11.965	1.00	41.18
ATOM	1471	O	GLY	A	494	33.916	16.011	12.747	1.00	38.22
ATOM	1472	N	LEU	A	495	32.905	14.138	12.043	1.00	39.53
ATOM	1473	CA	LEU	A	495	31.876	14.248	13.068	1.00	38.91
ATOM	1474	CB	LEU	A	495	30.713	13.304	12.769	1.00	39.20
ATOM	1475	CG	LEU	A	495	29.540	13.901	11.988	1.00	40.73

ATOM	1476	CD1	LEU	A	495	29.976	14.170	10.553	1.00	37.80
ATOM	1477	CD2	LEU	A	495	28.349	12.943	12.026	1.00	40.94
ATOM	1478	C	LEU	A	495	32.461	13.923	14.431	1.00	36.01
ATOM	1479	O	LEU	A	495	33.347	13.074	14.544	1.00	34.85
ATOM	1480	N	THR	A	496	31.979	14.604	15.459	1.00	37.52
ATOM	1481	CA	THR	A	496	32.462	14.350	16.812	1.00	35.45
ATOM	1482	CB	THR	A	496	31.925	15.375	17.829	1.00	37.55
ATOM	1483	OG1	THR	A	496	30.498	15.263	17.908	1.00	32.93
ATOM	1484	CG2	THR	A	496	32.315	16.797	17.434	1.00	36.16
ATOM	1485	C	THR	A	496	31.933	12.987	17.210	1.00	35.67
ATOM	1486	O	THR	A	496	31.081	12.427	16.521	1.00	34.34
ATOM	1487	N	LEU	A	497	32.429	12.452	18.319	1.00	34.88
ATOM	1488	CA	LEU	A	497	31.965	11.151	18.786	1.00	35.67
ATOM	1489	CB	LEU	A	497	32.689	10.760	20.074	1.00	41.10
ATOM	1490	CG	LEU	A	497	33.714	9.640	19.896	1.00	45.27
ATOM	1491	CD1	LEU	A	497	34.755	9.692	21.008	1.00	45.09
ATOM	1492	CD2	LEU	A	497	32.988	8.305	19.884	1.00	47.77
ATOM	1493	C	LEU	A	497	30.455	11.198	19.026	1.00	33.72
ATOM	1494	O	LEU	A	497	29.712	10.350	18.534	1.00	33.20
ATOM	1495	N	GLN	A	498	30.006	12.202	19.773	1.00	30.82
ATOM	1496	CA	GLN	A	498	28.586	12.348	20.062	1.00	31.47
ATOM	1497	CB	GLN	A	498	28.344	13.566	20.951	1.00	30.51
ATOM	1498	CG	GLN	A	498	26.894	13.796	21.341	1.00	34.38
ATOM	1499	CD	GLN	A	498	26.712	15.130	22.015	1.00	38.60
ATOM	1500	OE1	GLN	A	498	27.363	16.112	21.686	1.00	42.92
ATOM	1501	NE2	GLN	A	498	25.809	15.176	23.008	1.00	40.02
ATOM	1502	C	GLN	A	498	27.776	12.476	18.773	1.00	30.47
ATOM	1503	O	GLN	A	498	26.682	11.927	18.665	1.00	30.85
ATOM	1504	N	GLN	A	499	28.311	13.196	17.793	1.00	29.52
ATOM	1505	CA	GLN	A	499	27.603	13.362	16.524	1.00	30.24
ATOM	1506	CB	GLN	A	499	28.292	14.420	15.661	1.00	30.20
ATOM	1507	CG	GLN	A	499	28.135	15.840	16.191	1.00	31.60
ATOM	1508	CD	GLN	A	499	28.930	16.849	15.389	1.00	31.61
ATOM	1509	OE1	GLN	A	499	29.956	16.518	14.795	1.00	30.66
ATOM	1510	NE2	GLN	A	499	28.457	18.089	15.364	1.00	34.17
ATOM	1511	C	GLN	A	499	27.529	12.047	15.753	1.00	29.40
ATOM	1512	O	GLN	A	499	26.567	11.793	15.032	1.00	30.04
ATOM	1513	N	GLN	A	500	28.550	11.214	15.903	1.00	25.67
ATOM	1514	CA	GLN	A	500	28.577	9.937	15.216	1.00	29.30
ATOM	1515	CB	GLN	A	500	29.933	9.276	15.406	1.00	31.52
ATOM	1516	CG	GLN	A	500	31.012	9.839	14.508	1.00	33.05
ATOM	1517	CD	GLN	A	500	32.371	9.370	14.930	1.00	34.84
ATOM	1518	OE1	GLN	A	500	32.612	8.194	15.141	1.00	36.47
ATOM	1519	NE2	GLN	A	500	33.301	10.324	15.082	1.00	38.25
ATOM	1520	C	GLN	A	500	27.459	9.017	15.711	1.00	27.98
ATOM	1521	O	GLN	A	500	26.700	8.469	14.908	1.00	24.84
ATOM	1522	N	HIS	A	501	27.357	8.864	17.029	1.00	26.20
ATOM	1523	CA	HIS	A	501	26.327	8.021	17.631	1.00	27.63

	ATOM	1524	CB	HIS	A	501	26.535	7.919	19.145	1.00	27.97
	ATOM	1525	CG	HIS	A	501	27.892	7.420	19.535	1.00	34.27
	ATOM	1526	CD2	HIS	A	501	28.726	6.540	18.931	1.00	36.10
	ATOM	1527	ND1	HIS	A	501	28.541	7.844	20.676	1.00	31.81
	ATOM	1528	CE1	HIS	A	501	29.716	7.244	20.758	1.00	34.89
	ATOM	1529	NE2	HIS	A	501	29.854	6.448	19.712	1.00	37.46
	ATOM	1530	C	HIS	A	501	24.935	8.572	17.348	1.00	24.93
	ATOM	1531	O	HIS	A	501	23.998	7.815	17.107	1.00	26.73
	ATOM	1532	N	GLN	A	502	24.796	9.892	17.379	1.00	22.79
	ATOM	1533	CA	GLN	A	502	23.504	10.498	17.119	1.00	26.14
	ATOM	1534	CB	GLN	A	502	23.554	12.006	17.371	1.00	22.36
	ATOM	1535	CG	GLN	A	502	23.460	12.378	18.848	1.00	26.19
	ATOM	1536	CD	GLN	A	502	23.589	13.875	19.089	1.00	28.67
	ATOM	1537	OE1	GLN	A	502	23.632	14.663	18.149	1.00	28.40
	ATOM	1538	NE2	GLN	A	502	23.651	14.268	20.355	1.00	24.72
	ATOM	1539	C	GLN	A	502	23.056	10.221	15.685	1.00	26.19
	ATOM	1540	O	GLN	A	502	21.913	9.822	15.453	1.00	24.09
	ATOM	1541	N	ARG	A	503	23.955	10.429	14.727	1.00	24.88
	ATOM	1542	CA	ARG	A	503	23.630	10.196	13.326	1.00	25.25
	ATOM	1543	CB	ARG	A	503	24.772	10.668	12.418	1.00	27.63
	ATOM	1544	CG	ARG	A	503	24.432	10.563	10.932	1.00	28.75
	ATOM	1545	CD	ARG	A	503	25.479	11.222	10.056	1.00	27.72
	ATOM	1546	NE	ARG	A	503	25.072	11.214	8.654	1.00	29.35
	ATOM	1547	CZ	ARG	A	503	24.279	12.126	8.105	1.00	25.84
	ATOM	1548	NH1	ARG	A	503	23.804	13.120	8.840	1.00	27.35
	ATOM	1549	NH2	ARG	A	503	23.962	12.044	6.820	1.00	30.63
	ATOM	1550	C	ARG	A	503	23.347	8.716	13.065	1.00	24.53
	ATOM	1551	O	ARG	A	503	22.425	8.375	12.321	1.00	25.90
	ATOM	1552	N	LEU	A	504	24.143	7.841	13.672	1.00	23.00
	ATOM	1553	CA	LEU	A	504	23.953	6.406	13.496	1.00	22.60
	ATOM	1554	CB	LEU	A	504	24.971	5.621	14.323	1.00	25.43
	ATOM	1555	CG	LEU	A	504	24.781	4.100	14.344	1.00	25.23
	ATOM	1556	CD1	LEU	A	504	25.166	3.505	12.991	1.00	28.52
	ATOM	1557	CD2	LEU	A	504	25.627	3.495	15.444	1.00	22.14
	ATOM	1558	C	LEU	A	504	22.541	6.030	13.934	1.00	22.84
	ATOM	1559	O	LEU	A	504	21.846	5.288	13.245	1.00	21.51
	ATOM	1560	N	ALA	A	505	22.120	6.547	15.083	1.00	20.16
	ATOM	1561	CA	ALA	A	505	20.784	6.262	15.585	1.00	21.08
	ATOM	1562	CB	ALA	A	505	20.605	6.868	16.980	1.00	23.57
	ATOM	1563	C	ALA	A	505	19.738	6.832	14.628	1.00	20.20
	ATOM	1564	O	ALA	A	505	18.754	6.164	14.293	1.00	17.31
	ATOM	1565	N	GLN	A	506	19.954	8.066	14.184	1.00	22.11
	ATOM	1566	CA	GLN	A	506	19.013	8.711	13.277	1.00	21.70
	ATOM	1567	CB	GLN	A	506	19.502	10.111	12.903	1.00	22.26
	ATOM	1568	CG	GLN	A	506	19.240	11.158	13.975	1.00	25.84
	ATOM	1569	CD	GLN	A	506	20.187	12.333	13.857	1.00	32.88
	ATOM	1570	OE1	GLN	A	506	20.704	12.614	12.777	1.00	31.23
	ATOM	1571	NE2	GLN	A	506	20.423	13.025	14.968	1.00	32.97

ATOM	1572	C	GLN	A	506	18.813	7.881	12.016	1.00	23.57
ATOM	1573	O	GLN	A	506	17.684	7.715	11.550	1.00	21.83
ATOM	1574	N	LEU	A	507	19.905	7.354	11.474	1.00	19.98
ATOM	1575	CA	LEU	A	507	19.827	6.537	10.263	1.00	22.03
ATOM	1576	CB	LEU	A	507	21.231	6.244	9.725	1.00	23.02
ATOM	1577	CG	LEU	A	507	22.026	7.457	9.225	1.00	25.80
ATOM	1578	CD1	LEU	A	507	23.371	6.994	8.713	1.00	27.67
ATOM	1579	CD2	LEU	A	507	21.264	8.176	8.130	1.00	25.62
ATOM	1580	C	LEU	A	507	19.090	5.219	10.496	1.00	22.35
ATOM	1581	O	LEU	A	507	18.242	4.825	9.695	1.00	19.33
ATOM	1582	N	LEU	A	508	19.402	4.539	11.592	1.00	21.29
ATOM	1583	CA	LEU	A	508	18.755	3.260	11.881	1.00	20.72
ATOM	1584	CB	LEU	A	508	19.501	2.535	13.001	1.00	22.29
ATOM	1585	CG	LEU	A	508	20.977	2.311	12.678	1.00	24.70
ATOM	1586	CD1	LEU	A	508	21.642	1.551	13.814	1.00	21.37
ATOM	1587	CD2	LEU	A	508	21.095	1.542	11.367	1.00	27.88
ATOM	1588	C	LEU	A	508	17.279	3.396	12.239	1.00	19.14
ATOM	1589	O	LEU	A	508	16.498	2.478	12.003	1.00	17.80
ATOM	1590	N	LEU	A	509	16.895	4.530	12.815	1.00	19.23
ATOM	1591	CA	LEU	A	509	15.495	4.747	13.173	1.00	20.14
ATOM	1592	CB	LEU	A	509	15.347	6.030	13.999	1.00	20.28
ATOM	1593	CG	LEU	A	509	15.710	5.858	15.479	1.00	21.35
ATOM	1594	CD1	LEU	A	509	15.354	7.106	16.263	1.00	19.29
ATOM	1595	CD2	LEU	A	509	14.989	4.656	16.038	1.00	20.84
ATOM	1596	C	LEU	A	509	14.681	4.841	11.885	1.00	21.69
ATOM	1597	O	LEU	A	509	13.493	4.514	11.854	1.00	22.40
ATOM	1598	N	ILE	A	510	15.343	5.270	10.815	1.00	20.22
ATOM	1599	CA	ILE	A	510	14.710	5.397	9.508	1.00	20.40
ATOM	1600	CB	ILE	A	510	15.720	5.946	8.464	1.00	28.34
ATOM	1601	CG2	ILE	A	510	15.208	5.710	7.056	1.00	32.54
ATOM	1602	CG1	ILE	A	510	15.965	7.438	8.696	1.00	28.23
ATOM	1603	CD1	ILE	A	510	14.789	8.189	9.288	1.00	33.16
ATOM	1604	C	ILE	A	510	14.210	4.025	9.049	1.00	23.21
ATOM	1605	O	ILE	A	510	13.120	3.906	8.474	1.00	21.16
ATOM	1606	N	LEU	A	511	14.998	2.989	9.323	1.00	18.38
ATOM	1607	CA	LEU	A	511	14.633	1.634	8.917	1.00	20.10
ATOM	1608	CB	LEU	A	511	15.754	0.656	9.267	1.00	21.69
ATOM	1609	CG	LEU	A	511	17.128	1.022	8.692	1.00	26.03
ATOM	1610	CD1	LEU	A	511	18.024	-0.206	8.724	1.00	22.68
ATOM	1611	CD2	LEU	A	511	16.996	1.544	7.267	1.00	26.00
ATOM	1612	C	LEU	A	511	13.326	1.181	9.543	1.00	18.51
ATOM	1613	O	LEU	A	511	12.663	0.283	9.025	1.00	17.40
ATOM	1614	N	SER	A	512	12.963	1.799	10.664	1.00	18.68
ATOM	1615	CA	SER	A	512	11.718	1.471	11.331	1.00	18.67
ATOM	1616	CB	SER	A	512	11.661	2.117	12.720	1.00	18.58
ATOM	1617	OG	SER	A	512	10.315	2.229	13.165	1.00	27.92
ATOM	1618	C	SER	A	512	10.572	1.994	10.464	1.00	18.43
ATOM	1619	O	SER	A	512	9.584	1.296	10.236	1.00	13.91

	ATOM	1620	N	HIS	A	513	10.713	3.228	9.982	1.00	18.95
	ATOM	1621	CA	HIS	A	513	9.698	3.831	9.124	1.00	20.82
	ATOM	1622	CB	HIS	A	513	10.013	5.315	8.894	1.00	24.36
	ATOM	1623	CG	HIS	A	513	9.923	6.146	10.136	1.00	32.13
5	ATOM	1624	CD2	HIS	A	513	8.863	6.744	10.734	1.00	35.29
	ATOM	1625	ND1	HIS	A	513	11.010	6.391	10.949	1.00	35.00
	ATOM	1626	CE1	HIS	A	513	10.624	7.101	11.995	1.00	34.67
	ATOM	1627	NE2	HIS	A	513	9.326	7.328	11.889	1.00	35.82
	ATOM	1628	C	HIS	A	513	9.650	3.079	7.790	1.00	19.08
10	ATOM	1629	O	HIS	A	513	8.575	2.863	7.220	1.00	21.20
	ATOM	1630	N	ILE	A	514	10.809	2.662	7.297	1.00	15.58
	ATOM	1631	CA	ILE	A	514	10.849	1.921	6.038	1.00	16.48
	ATOM	1632	CB	ILE	A	514	12.312	1.678	5.576	1.00	20.09
	ATOM	1633	CG2	ILE	A	514	12.349	0.602	4.499	1.00	19.55
15	ATOM	1634	CG1	ILE	A	514	12.891	2.986	5.019	1.00	22.62
	ATOM	1635	CD1	ILE	A	514	14.393	2.992	4.874	1.00	27.34
	ATOM	1636	C	ILE	A	514	10.112	0.590	6.210	1.00	16.40
	ATOM	1637	O	ILE	A	514	9.364	0.164	5.328	1.00	17.91
	ATOM	1638	N	ARG	A	515	10.301	-0.071	7.347	1.00	18.20
20	ATOM	1639	CA	ARG	A	515	9.585	-1.327	7.564	1.00	18.05
	ATOM	1640	CB	ARG	A	515	9.984	-1.980	8.889	1.00	18.36
	ATOM	1641	CG	ARG	A	515	9.173	-3.237	9.213	1.00	17.84
	ATOM	1642	CD	ARG	A	515	9.823	-4.470	8.606	1.00	17.94
	ATOM	1643	NE	ARG	A	515	11.038	-4.813	9.334	1.00	26.96
25	ATOM	1644	CZ	ARG	A	515	11.406	-6.051	9.641	1.00	25.13
	ATOM	1645	NH1	ARG	A	515	10.654	-7.080	9.281	1.00	23.49
	ATOM	1646	NH2	ARG	A	515	12.511	-6.254	10.340	1.00	32.16
	ATOM	1647	C	ARG	A	515	8.089	-1.020	7.594	1.00	18.29
	ATOM	1648	O	ARG	A	515	7.275	-1.759	7.038	1.00	16.22
30	ATOM	1649	N	HIS	A	516	7.726	0.085	8.237	1.00	19.33
	ATOM	1650	CA	HIS	A	516	6.317	0.441	8.330	1.00	17.78
	ATOM	1651	CB	HIS	A	516	6.126	1.702	9.166	1.00	16.84
	ATOM	1652	CG	HIS	A	516	4.692	2.101	9.312	1.00	18.16
	ATOM	1653	CD2	HIS	A	516	3.967	3.061	8.691	1.00	21.17
35	ATOM	1654	ND1	HIS	A	516	3.830	1.469	10.180	1.00	20.70
	ATOM	1655	CE1	HIS	A	516	2.633	2.022	10.089	1.00	21.52
	ATOM	1656	NE2	HIS	A	516	2.689	2.992	9.191	1.00	20.16
	ATOM	1657	C	HIS	A	516	5.708	0.659	6.954	1.00	16.63
	ATOM	1658	O	HIS	A	516	4.598	0.216	6.689	1.00	18.58
40	ATOM	1659	N	MET	A	517	6.438	1.334	6.073	1.00	15.29
	ATOM	1660	CA	MET	A	517	5.925	1.589	4.730	1.00	16.58
	ATOM	1661	CB	MET	A	517	6.837	2.576	4.002	1.00	18.66
	ATOM	1662	CG	MET	A	517	6.805	3.978	4.631	1.00	16.88
	ATOM	1663	SD	MET	A	517	7.670	5.243	3.701	1.00	24.08
45	ATOM	1664	CE	MET	A	517	9.390	4.777	3.962	1.00	14.30
	ATOM	1665	C	MET	A	517	5.773	0.289	3.940	1.00	17.86
	ATOM	1666	O	MET	A	517	4.791	0.101	3.224	1.00	18.25
	ATOM	1667	N	SER	A	518	6.741	-0.610	4.086	1.00	17.43

	ATOM	1668	CA	SER	A	518	6.697	-1.896	3.403	1.00	18.40
	ATOM	1669	CB	SER	A	518	7.974	-2.695	3.680	1.00	16.77
	ATOM	1670	OG	SER	A	518	7.834	-4.030	3.227	1.00	24.23
	ATOM	1671	C	SER	A	518	5.476	-2.695	3.854	1.00	17.91
5	ATOM	1672	O	SER	A	518	4.788	-3.295	3.030	1.00	18.97
	ATOM	1673	N	ASN	A	519	5.204	-2.697	5.159	1.00	21.82
	ATOM	1674	CA	ASN	A	519	4.047	-3.418	5.696	1.00	21.99
	ATOM	1675	CB	ASN	A	519	3.957	-3.257	7.216	1.00	23.24
	ATOM	1676	CG	ASN	A	519	5.046	-4.011	7.957	1.00	31.14
10	ATOM	1677	OD1	ASN	A	519	5.585	-4.999	7.461	1.00	32.50
	ATOM	1678	ND2	ASN	A	519	5.368	-3.545	9.163	1.00	29.10
	ATOM	1679	C	ASN	A	519	2.761	-2.871	5.079	1.00	23.76
	ATOM	1680	O	ASN	A	519	1.902	-3.632	4.631	1.00	24.48
	ATOM	1681	N	LYS	A	520	2.627	-1.548	5.078	1.00	20.58
15	ATOM	1682	CA	LYS	A	520	1.449	-0.900	4.512	1.00	25.49
	ATOM	1683	CB	LYS	A	520	1.484	0.607	4.786	1.00	24.73
	ATOM	1684	CG	LYS	A	520	1.512	0.996	6.264	1.00	32.31
	ATOM	1685	CD	LYS	A	520	0.656	0.080	7.133	1.00	37.11
	ATOM	1686	CE	LYS	A	520	-0.787	0.547	7.181	1.00	41.56
20	ATOM	1687	NZ	LYS	A	520	-1.560	-0.134	8.261	1.00	42.66
	ATOM	1688	C	LYS	A	520	1.380	-1.144	3.005	1.00	25.40
	ATOM	1689	O	LYS	A	520	0.316	-1.436	2.467	1.00	26.44
	ATOM	1690	N	GLY	A	521	2.520	-1.021	2.332	1.00	22.88
	ATOM	1691	CA	GLY	A	521	2.561	-1.236	0.897	1.00	21.53
25	ATOM	1692	C	GLY	A	521	2.177	-2.655	0.536	1.00	24.79
	ATOM	1693	O	GLY	A	521	1.426	-2.878	-0.413	1.00	25.71
	ATOM	1694	N	MET	A	522	2.696	-3.619	1.290	1.00	22.75
	ATOM	1695	CA	MET	A	522	2.393	-5.027	1.058	1.00	23.40
	ATOM	1696	CB	MET	A	522	3.170	-5.898	2.042	1.00	25.74
30	ATOM	1697	CG	MET	A	522	3.396	-7.308	1.559	1.00	31.06
	ATOM	1698	SD	MET	A	522	4.572	-7.352	0.202	1.00	34.06
	ATOM	1699	CE	MET	A	522	6.125	-7.229	1.113	1.00	29.28
	ATOM	1700	C	MET	A	522	0.893	-5.281	1.218	1.00	26.49
	ATOM	1701	O	MET	A	522	0.268	-5.920	0.361	1.00	25.47
35	ATOM	1702	N	GLU	A	523	0.321	-4.790	2.318	1.00	24.95
	ATOM	1703	CA	GLU	A	523	-1.110	-4.954	2.566	1.00	27.15
	ATOM	1704	CB	GLU	A	523	-1.555	-4.206	3.835	1.00	31.08
	ATOM	1705	CG	GLU	A	523	-0.830	-4.564	5.124	1.00	38.93
	ATOM	1706	CD	GLU	A	523	-1.153	-3.585	6.258	1.00	46.90
40	ATOM	1707	OE1	GLU	A	523	-2.225	-2.938	6.200	1.00	47.40
	ATOM	1708	OE2	GLU	A	523	-0.337	-3.460	7.202	1.00	47.39
	ATOM	1709	C	GLU	A	523	-1.872	-4.368	1.381	1.00	26.10
	ATOM	1710	O	GLU	A	523	-2.817	-4.964	0.882	1.00	24.25
	ATOM	1711	N	HIS	A	524	-1.449	-3.182	0.940	1.00	24.74
45	ATOM	1712	CA	HIS	A	524	-2.093	-2.505	-0.173	1.00	26.17
	ATOM	1713	CB	HIS	A	524	-1.481	-1.125	-0.379	1.00	24.64
	ATOM	1714	CG	HIS	A	524	-2.233	-0.278	-1.355	1.00	30.59
	ATOM	1715	CD2	HIS	A	524	-3.227	0.624	-1.172	1.00	32.15

	ATOM	1716	ND1	HIS	A	524	-2.008	-0.332	-2.713	1.00	27.46
	ATOM	1717	CE1	HIS	A	524	-2.829	0.502	-3.326	1.00	34.58
	ATOM	1718	NE2	HIS	A	524	-3.580	1.094	-2.413	1.00	30.50
	ATOM	1719	C	HIS	A	524	-1.996	-3.294	-1.474	1.00	28.06
	ATOM	1720	O	HIS	A	524	-2.976	-3.419	-2.217	1.00	29.81
	ATOM	1721	N	LEU	A	525	-0.811	-3.824	-1.746	1.00	27.07
	ATOM	1722	CA	LEU	A	525	-0.594	-4.601	-2.955	1.00	29.30
	ATOM	1723	CB	LEU	A	525	0.865	-5.039	-3.051	1.00	26.39
	ATOM	1724	CG	LEU	A	525	1.307	-5.765	-4.321	1.00	29.34
	ATOM	1725	CD1	LEU	A	525	0.734	-5.076	-5.562	1.00	29.61
	ATOM	1726	CD2	LEU	A	525	2.829	-5.769	-4.370	1.00	29.22
	ATOM	1727	C	LEU	A	525	-1.497	-5.822	-2.950	1.00	31.67
	ATOM	1728	O	LEU	A	525	-2.128	-6.133	-3.957	1.00	32.45
	ATOM	1729	N	TYR	A	526	-1.559	-6.512	-1.814	1.00	36.14
	ATOM	1730	CA	TYR	A	526	-2.397	-7.698	-1.696	1.00	40.36
	ATOM	1731	CB	TYR	A	526	-2.221	-8.350	-0.324	1.00	45.27
	ATOM	1732	CG	TYR	A	526	-2.849	-9.722	-0.229	1.00	50.62
	ATOM	1733	CD1	TYR	A	526	-2.114	-10.867	-0.537	1.00	54.55
	ATOM	1734	CE1	TYR	A	526	-2.698	-12.136	-0.482	1.00	57.27
	ATOM	1735	CD2	TYR	A	526	-4.188	-9.876	0.142	1.00	53.48
	ATOM	1736	CE2	TYR	A	526	-4.781	-11.141	0.201	1.00	55.93
	ATOM	1737	CZ	TYR	A	526	-4.029	-12.264	-0.113	1.00	56.60
	ATOM	1738	OH	TYR	A	526	-4.603	-13.515	-0.063	1.00	60.70
	ATOM	1739	C	TYR	A	526	-3.852	-7.298	-1.893	1.00	42.83
	ATOM	1740	O	TYR	A	526	-4.673	-8.094	-2.349	1.00	43.49
	ATOM	1741	N	SER	A	527	-4.158	-6.055	-1.543	1.00	41.55
	ATOM	1742	CA	SER	A	527	-5.503	-5.523	-1.686	1.00	44.04
	ATOM	1743	CB	SER	A	527	-5.606	-4.169	-0.979	1.00	43.47
	ATOM	1744	OG	SER	A	527	-6.954	-3.789	-0.786	1.00	47.51
	ATOM	1745	C	SER	A	527	-5.817	-5.356	-3.172	1.00	44.18
	ATOM	1746	O	SER	A	527	-6.883	-5.757	-3.642	1.00	44.88
	ATOM	1747	N	MET	A	528	-4.883	-4.755	-3.901	1.00	41.79
	ATOM	1748	CA	MET	A	528	-5.047	-4.536	-5.331	1.00	44.04
	ATOM	1749	CB	MET	A	528	-3.898	-3.679	-5.870	1.00	44.78
	ATOM	1750	CG	MET	A	528	-3.965	-2.206	-5.468	1.00	45.37
	ATOM	1751	SD	MET	A	528	-5.652	-1.598	-5.273	1.00	51.83
	ATOM	1752	CE	MET	A	528	-5.553	-0.004	-6.044	1.00	46.61
	ATOM	1753	C	MET	A	528	-5.087	-5.871	-6.071	1.00	44.29
	ATOM	1754	O	MET	A	528	-5.689	-5.979	-7.137	1.00	44.02
	ATOM	1755	N	LYS	A	529	-4.443	-6.883	-5.499	1.00	46.78
	ATOM	1756	CA	LYS	A	529	-4.413	-8.213	-6.099	1.00	51.28
	ATOM	1757	CB	LYS	A	529	-3.550	-9.158	-5.261	1.00	50.87
	ATOM	1758	CG	LYS	A	529	-2.798	-10.204	-6.071	1.00	50.55
	ATOM	1759	CD	LYS	A	529	-3.548	-11.520	-6.104	1.00	51.25
	ATOM	1760	CE	LYS	A	529	-2.616	-12.694	-5.856	1.00	53.22
	ATOM	1761	NZ	LYS	A	529	-2.420	-12.954	-4.402	1.00	53.22
	ATOM	1762	C	LYS	A	529	-5.829	-8.768	-6.182	1.00	54.27
	ATOM	1763	O	LYS	A	529	-6.325	-9.069	-7.266	1.00	55.50

ATOM	1764	N	CYS	A	530	-6.472	-8.901	-5.027	1.00	56.71
ATOM	1765	CA	CYS	A	530	-7.833	-9.416	-4.961	1.00	58.35
ATOM	1766	CB	CYS	A	530	-8.333	-9.380	-3.517	1.00	59.78
ATOM	1767	SG	CYS	A	530	-7.289	-10.304	-2.358	1.00	63.19
ATOM	1768	C	CYS	A	530	-8.766	-8.609	-5.858	1.00	59.36
ATOM	1769	O	CYS	A	530	-9.644	-9.169	-6.514	1.00	59.52
ATOM	1770	N	LYS	A	531	-8.569	-7.293	-5.888	1.00	59.24
ATOM	1771	CA	LYS	A	531	-9.390	-6.411	-6.713	1.00	60.14
ATOM	1772	CB	LYS	A	531	-9.158	-4.952	-6.317	1.00	58.92
ATOM	1773	C	LYS	A	531	-9.073	-6.615	-8.195	1.00	61.48
ATOM	1774	O	LYS	A	531	-9.618	-5.928	-9.061	1.00	61.74
ATOM	1775	N	ASN	A	532	-8.179	-7.561	-8.474	1.00	61.65
ATOM	1776	CA	ASN	A	532	-7.783	-7.890	-9.840	1.00	61.60
ATOM	1777	CB	ASN	A	532	-8.966	-8.518	-10.581	1.00	62.28
ATOM	1778	CG	ASN	A	532	-8.750	-9.985	-10.878	1.00	64.66
ATOM	1779	OD1	ASN	A	532	-8.344	-10.352	-11.983	1.00	67.08
ATOM	1780	ND2	ASN	A	532	-9.016	-10.836	-9.891	1.00	62.68
ATOM	1781	C	ASN	A	532	-7.247	-6.710	-10.648	1.00	59.75
ATOM	1782	O	ASN	A	532	-7.487	-6.615	-11.850	1.00	57.50
ATOM	1783	N	VAL	A	533	-6.507	-5.822	-9.992	1.00	59.39
ATOM	1784	CA	VAL	A	533	-5.954	-4.656	-10.669	1.00	58.22
ATOM	1785	CB	VAL	A	533	-6.223	-3.371	-9.865	1.00	59.20
ATOM	1786	CG1	VAL	A	533	-6.181	-2.163	-10.785	1.00	59.21
ATOM	1787	CG2	VAL	A	533	-7.574	-3.467	-9.172	1.00	59.57
ATOM	1788	C	VAL	A	533	-4.452	-4.767	-10.907	1.00	57.86
ATOM	1789	O	VAL	A	533	-3.846	-3.874	-11.499	1.00	60.56
ATOM	1790	N	VAL	A	534	-3.852	-5.863	-10.451	1.00	56.03
ATOM	1791	CA	VAL	A	534	-2.417	-6.063	-10.621	1.00	54.11
ATOM	1792	CB	VAL	A	534	-1.767	-6.632	-9.341	1.00	54.02
ATOM	1793	CG1	VAL	A	534	-0.300	-6.950	-9.601	1.00	52.37
ATOM	1794	CG2	VAL	A	534	-1.900	-5.635	-8.200	1.00	55.70
ATOM	1795	C	VAL	A	534	-2.089	-7.008	-11.770	1.00	54.31
ATOM	1796	O	VAL	A	534	-2.519	-8.164	-11.780	1.00	51.66
ATOM	1797	N	PRO	A	535	-1.315	-6.527	-12.755	1.00	53.54
ATOM	1798	CD	PRO	A	535	-0.749	-5.172	-12.874	1.00	54.28
ATOM	1799	CA	PRO	A	535	-0.949	-7.373	-13.893	1.00	53.24
ATOM	1800	CB	PRO	A	535	0.011	-6.500	-14.697	1.00	52.71
ATOM	1801	CG	PRO	A	535	-0.353	-5.102	-14.319	1.00	53.19
ATOM	1802	C	PRO	A	535	-0.296	-8.664	-13.411	1.00	54.25
ATOM	1803	O	PRO	A	535	0.121	-8.768	-12.254	1.00	54.56
ATOM	1804	N	LEU	A	536	-0.203	-9.645	-14.299	1.00	53.63
ATOM	1805	CA	LEU	A	536	0.382	-10.926	-13.937	1.00	53.11
ATOM	1806	CB	LEU	A	536	-0.250	-12.046	-14.763	1.00	51.88
ATOM	1807	CG	LEU	A	536	-0.686	-13.256	-13.938	1.00	51.83
ATOM	1808	CD1	LEU	A	536	-1.953	-12.917	-13.173	1.00	49.51
ATOM	1809	CD2	LEU	A	536	-0.905	-14.449	-14.854	1.00	53.43
ATOM	1810	C	LEU	A	536	1.895	-10.990	-14.081	1.00	52.58
ATOM	1811	O	LEU	A	536	2.414	-11.501	-15.075	1.00	55.33

ATOM	1812	N	TYR	A	537	2.601	-10.462	-13.087	1.00	48.72
ATOM	1813	CA	TYR	A	537	4.057	-10.501	-13.093	1.00	44.22
ATOM	1814	CB	TYR	A	537	4.627	-9.134	-12.709	1.00	44.52
ATOM	1815	CG	TYR	A	537	4.331	-8.053	-13.731	1.00	45.18
ATOM	1816	CD1	TYR	A	537	3.623	-6.905	-13.376	1.00	43.77
ATOM	1817	CE1	TYR	A	537	3.334	-5.915	-14.317	1.00	45.23
ATOM	1818	CD2	TYR	A	537	4.747	-8.187	-15.058	1.00	46.91
ATOM	1819	CE2	TYR	A	537	4.462	-7.202	-16.008	1.00	43.93
ATOM	1820	CZ	TYR	A	537	3.757	-6.071	-15.631	1.00	46.70
ATOM	1821	OH	TYR	A	537	3.472	-5.097	-16.565	1.00	48.35
ATOM	1822	C	TYR	A	537	4.401	-11.562	-12.056	1.00	41.29
ATOM	1823	O	TYR	A	537	4.330	-11.319	-10.856	1.00	41.82
ATOM	1824	N	ASP	A	538	4.748	-12.748	-12.540	1.00	40.34
ATOM	1825	CA	ASP	A	538	5.055	-13.896	-11.691	1.00	38.84
ATOM	1826	CB	ASP	A	538	5.594	-15.037	-12.554	1.00	43.47
ATOM	1827	CG	ASP	A	538	4.571	-15.531	-13.566	1.00	47.67
ATOM	1828	OD1	ASP	A	538	4.931	-16.373	-14.416	1.00	49.33
ATOM	1829	OD2	ASP	A	538	3.405	-15.073	-13.511	1.00	48.07
ATOM	1830	C	ASP	A	538	5.991	-13.676	-10.508	1.00	37.28
ATOM	1831	O	ASP	A	538	5.620	-13.964	-9.371	1.00	38.55
ATOM	1832	N	LEU	A	539	7.196	-13.200	-10.766	1.00	33.83
ATOM	1833	CA	LEU	A	539	8.155	-12.959	-9.692	1.00	32.80
ATOM	1834	CB	LEU	A	539	9.419	-12.323	-10.263	1.00	32.78
ATOM	1835	CG	LEU	A	539	10.561	-12.031	-9.292	1.00	30.93
ATOM	1836	CD1	LEU	A	539	10.913	-13.280	-8.492	1.00	33.81
ATOM	1837	CD2	LEU	A	539	11.758	-11.538	-10.077	1.00	25.92
ATOM	1838	C	LEU	A	539	7.558	-12.050	-8.614	1.00	31.85
ATOM	1839	O	LEU	A	539	7.590	-12.367	-7.423	1.00	25.63
ATOM	1840	N	LEU	A	540	7.011	-10.917	-9.042	1.00	32.07
ATOM	1841	CA	LEU	A	540	6.411	-9.976	-8.111	1.00	31.03
ATOM	1842	CB	LEU	A	540	5.792	-8.800	-8.861	1.00	30.56
ATOM	1843	CG	LEU	A	540	5.124	-7.774	-7.945	1.00	31.12
ATOM	1844	CD1	LEU	A	540	6.092	-7.357	-6.838	1.00	29.76
ATOM	1845	CD2	LEU	A	540	4.693	-6.572	-8.762	1.00	30.85
ATOM	1846	C	LEU	A	540	5.337	-10.660	-7.282	1.00	34.55
ATOM	1847	O	LEU	A	540	5.316	-10.522	-6.063	1.00	31.60
ATOM	1848	N	LEU	A	541	4.446	-11.388	-7.941	1.00	35.64
ATOM	1849	CA	LEU	A	541	3.378	-12.101	-7.245	1.00	37.84
ATOM	1850	CB	LEU	A	541	2.452	-12.771	-8.255	1.00	38.49
ATOM	1851	CG	LEU	A	541	1.244	-11.932	-8.678	1.00	39.80
ATOM	1852	CD1	LEU	A	541	0.476	-11.476	-7.448	1.00	40.02
ATOM	1853	CD2	LEU	A	541	1.713	-10.733	-9.485	1.00	40.48
ATOM	1854	C	LEU	A	541	3.937	-13.147	-6.275	1.00	40.10
ATOM	1855	O	LEU	A	541	3.472	-13.254	-5.137	1.00	42.72
ATOM	1856	N	GLU	A	542	4.929	-13.915	-6.723	1.00	38.45
ATOM	1857	CA	GLU	A	542	5.535	-14.932	-5.868	1.00	39.59
ATOM	1858	CB	GLU	A	542	6.738	-15.566	-6.564	1.00	41.73
ATOM	1859	CG	GLU	A	542	6.396	-16.327	-7.831	1.00	48.34

ATOM	1860	CD	GLU	A	542	6.931	-17.747	-7.819	1.00	52.57
ATOM	1861	OE1	GLU	A	542	8.049	-17.961	-7.298	1.00	52.70
ATOM	1862	OE2	GLU	A	542	6.230	-18.647	-8.331	1.00	53.69
ATOM	1863	C	GLU	A	542	5.989	-14.299	-4.553	1.00	39.94
ATOM	1864	O	GLU	A	542	5.567	-14.710	-3.472	1.00	40.99
ATOM	1865	N	MET	A	543	6.844	-13.287	-4.663	1.00	38.29
ATOM	1866	CA	MET	A	543	7.380	-12.580	-3.503	1.00	38.11
ATOM	1867	CB	MET	A	543	8.242	-11.408	-3.963	1.00	37.34
ATOM	1868	CG	MET	A	543	9.311	-11.797	-4.953	1.00	40.59
ATOM	1869	SD	MET	A	543	10.829	-12.223	-4.114	1.00	45.64
ATOM	1870	CE	MET	A	543	12.014	-11.399	-5.151	1.00	42.61
ATOM	1871	C	MET	A	543	6.287	-12.064	-2.581	1.00	37.94
ATOM	1872	O	MET	A	543	6.413	-12.127	-1.358	1.00	39.20
ATOM	1873	N	LEU	A	544	5.218	-11.544	-3.175	1.00	39.44
ATOM	1874	CA	LEU	A	544	4.100	-11.013	-2.408	1.00	40.91
ATOM	1875	CB	LEU	A	544	3.087	-10.344	-3.341	1.00	39.88
ATOM	1876	CG	LEU	A	544	1.775	-9.905	-2.688	1.00	42.70
ATOM	1877	CD1	LEU	A	544	2.060	-8.886	-1.586	1.00	37.35
ATOM	1878	CD2	LEU	A	544	0.854	-9.317	-3.741	1.00	38.47
ATOM	1879	C	LEU	A	544	3.420	-12.120	-1.614	1.00	42.83
ATOM	1880	O	LEU	A	544	2.957	-11.899	-0.496	1.00	42.73
ATOM	1881	N	ASP	A	545	3.367	-13.313	-2.197	1.00	46.32
ATOM	1882	CA	ASP	A	545	2.746	-14.456	-1.539	1.00	50.65
ATOM	1883	CB	ASP	A	545	2.606	-15.617	-2.524	1.00	53.67
ATOM	1884	CG	ASP	A	545	1.703	-15.278	-3.691	1.00	57.35
ATOM	1885	OD1	ASP	A	545	0.697	-14.568	-3.475	1.00	59.99
ATOM	1886	OD2	ASP	A	545	1.999	-15.718	-4.824	1.00	59.68
ATOM	1887	C	ASP	A	545	3.559	-14.898	-0.327	1.00	50.74
ATOM	1888	O	ASP	A	545	3.004	-15.388	0.657	1.00	49.39
ATOM	1889	N	ALA	A	546	4.874	-14.723	-0.401	1.00	51.82
ATOM	1890	CA	ALA	A	546	5.750	-15.095	0.702	1.00	53.12
ATOM	1891	CB	ALA	A	546	7.180	-14.678	0.395	1.00	53.19
ATOM	1892	C	ALA	A	546	5.269	-14.424	1.987	1.00	54.67
ATOM	1893	O	ALA	A	546	5.476	-14.940	3.085	1.00	52.32
ATOM	1894	N	HIS	A	547	4.622	-13.270	1.838	1.00	56.66
ATOM	1895	CA	HIS	A	547	4.102	-12.520	2.978	1.00	59.19
ATOM	1896	CB	HIS	A	547	4.144	-11.017	2.684	1.00	56.70
ATOM	1897	CG	HIS	A	547	5.489	-10.394	2.896	1.00	54.64
ATOM	1898	CD2	HIS	A	547	6.644	-10.506	2.199	1.00	53.92
ATOM	1899	ND1	HIS	A	547	5.748	-9.514	3.925	1.00	52.17
ATOM	1900	CE1	HIS	A	547	7.004	-9.111	3.853	1.00	52.16
ATOM	1901	NE2	HIS	A	547	7.570	-9.698	2.814	1.00	51.90
ATOM	1902	C	HIS	A	547	2.668	-12.940	3.306	1.00	62.77
ATOM	1903	O	HIS	A	547	1.842	-12.120	3.707	1.00	63.24
ATOM	1904	N	ARG	A	548	2.381	-14.224	3.133	1.00	68.37
ATOM	1905	CA	ARG	A	548	1.053	-14.758	3.411	1.00	72.75
ATOM	1906	CB	ARG	A	548	0.243	-14.864	2.113	1.00	73.73
ATOM	1907	CG	ARG	A	548	-1.149	-14.243	2.186	1.00	74.04

ATOM	1908	CD	ARG	A	548	-1.081	-12.728	2.297	1.00	74.50
ATOM	1909	NE	ARG	A	548	-2.305	-12.167	2.863	1.00	75.04
ATOM	1910	CZ	ARG	A	548	-2.478	-10.880	3.149	1.00	75.59
ATOM	1911	NH1	ARG	A	548	-1.506	-10.006	2.919	1.00	75.79
ATOM	1912	NH2	ARG	A	548	-3.627	-10.464	3.662	1.00	76.00
ATOM	1913	C	ARG	A	548	1.179	-16.133	4.061	1.00	74.94
ATOM	1914	O	ARG	A	548	0.197	-16.697	4.549	1.00	75.15
ATOM	1915	N	LEU	A	549	2.398	-16.665	4.063	1.00	76.49
ATOM	1916	CA	LEU	A	549	2.669	-17.969	4.653	1.00	78.14
ATOM	1917	CB	LEU	A	549	2.971	-18.986	3.557	1.00	77.55
ATOM	1918	C	LEU	A	549	3.846	-17.870	5.619	1.00	79.13
ATOM	1919	O	LEU	A	549	4.892	-17.317	5.215	1.00	80.40
ATOM	1920	OXT	LEU	A	549	3.708	-18.341	6.769	1.00	79.46
HETATM	1921	CP9	DES	A	600	5.390	-3.061	-6.139	1.00	21.38
HETATM	1922	CP8	DES	A	600	5.834	-1.989	-5.134	1.00	22.41
HETATM	1923	CP7	DES	A	600	5.038	-0.714	-5.236	1.00	21.32
HETATM	1924	CP6	DES	A	600	3.587	-0.864	-5.062	1.00	25.87
HETATM	1925	CP1	DES	A	600	2.987	-0.978	-3.784	1.00	23.92
HETATM	1926	CP2	DES	A	600	1.597	-1.150	-3.684	1.00	29.77
HETATM	1927	CP3	DES	A	600	0.842	-1.214	-4.871	1.00	31.40
HETATM	1928	OP3	DES	A	600	-0.506	-1.419	-4.824	1.00	33.36
HETATM	1929	CP4	DES	A	600	1.421	-1.099	-6.143	1.00	27.01
HETATM	1930	CP5	DES	A	600	2.793	-0.929	-6.230	1.00	27.40
HETATM	1931	C7	DES	A	600	5.671	0.461	-5.482	1.00	22.39
HETATM	1932	C6	DES	A	600	7.113	0.561	-5.809	1.00	21.75
HETATM	1933	C5	DES	A	600	7.541	0.306	-7.131	1.00	19.97
HETATM	1934	C4	DES	A	600	8.889	0.429	-7.477	1.00	23.81
HETATM	1935	C3	DES	A	600	9.814	0.804	-6.488	1.00	21.88
HETATM	1936	O3	DES	A	600	11.125	0.901	-6.839	1.00	22.32
HETATM	1937	C2	DES	A	600	9.423	1.066	-5.161	1.00	19.74
HETATM	1938	C1	DES	A	600	8.066	0.937	-4.838	1.00	21.25
HETATM	1939	C8	DES	A	600	4.894	1.765	-5.443	1.00	21.47
HETATM	1940	C9	DES	A	600	4.959	2.468	-4.070	1.00	21.38
HETATM	1941	CL	CL	A	601	14.781	-3.035	-17.739	1.00	24.10
ATOM	1942	CB	SER	B	305	12.321	21.086	25.295	1.00	64.27
ATOM	1943	C	SER	B	305	12.672	22.102	27.548	1.00	64.37
ATOM	1944	O	SER	B	305	13.701	22.760	27.702	1.00	66.90
ATOM	1945	N	SER	B	305	12.045	23.521	25.606	1.00	63.72
ATOM	1946	CA	SER	B	305	11.875	22.187	26.251	1.00	64.21
ATOM	1947	N	LEU	B	306	12.193	21.293	28.484	1.00	63.09
ATOM	1948	CA	LEU	B	306	12.884	21.133	29.757	1.00	60.98
ATOM	1949	CB	LEU	B	306	11.884	21.200	30.913	1.00	61.23
ATOM	1950	CG	LEU	B	306	12.221	20.417	32.183	1.00	62.23
ATOM	1951	CD1	LEU	B	306	13.304	21.144	32.966	1.00	62.56
ATOM	1952	CD2	LEU	B	306	10.965	20.258	33.027	1.00	64.31
ATOM	1953	C	LEU	B	306	13.660	19.819	29.803	1.00	58.39
ATOM	1954	O	LEU	B	306	14.570	19.654	30.614	1.00	58.56
ATOM	1955	N	ALA	B	307	13.293	18.881	28.933	1.00	54.82

	ATOM	1956	CA	ALA	B	307	13.971	17.589	28.861	1.00	50.62
	ATOM	1957	CB	ALA	B	307	13.092	16.584	28.143	1.00	51.30
	ATOM	1958	C	ALA	B	307	15.303	17.719	28.122	1.00	46.84
	ATOM	1959	O	ALA	B	307	16.196	16.885	28.274	1.00	45.62
	ATOM	1960	N	LEU	B	308	15.431	18.769	27.320	1.00	43.46
	ATOM	1961	CA	LEU	B	308	16.643	18.983	26.542	1.00	43.01
	ATOM	1962	CB	LEU	B	308	16.413	20.100	25.526	1.00	41.32
	ATOM	1963	CG	LEU	B	308	16.315	19.708	24.051	1.00	43.10
	ATOM	1964	CD1	LEU	B	308	15.942	18.239	23.903	1.00	40.51
	ATOM	1965	CD2	LEU	B	308	15.287	20.602	23.375	1.00	39.80
	ATOM	1966	C	LEU	B	308	17.874	19.297	27.385	1.00	42.11
	ATOM	1967	O	LEU	B	308	19.000	19.102	26.932	1.00	44.34
	ATOM	1968	N	SER	B	309	17.669	19.775	28.608	1.00	40.88
	ATOM	1969	CA	SER	B	309	18.796	20.100	29.475	1.00	42.79
	ATOM	1970	CB	SER	B	309	18.562	21.447	30.163	1.00	41.25
	ATOM	1971	OG	SER	B	309	17.459	21.379	31.046	1.00	46.67
	ATOM	1972	C	SER	B	309	19.072	19.028	30.529	1.00	42.60
	ATOM	1973	O	SER	B	309	20.053	19.119	31.269	1.00	44.18
	ATOM	1974	N	LEU	B	310	18.217	18.012	30.596	1.00	39.44
	ATOM	1975	CA	LEU	B	310	18.394	16.936	31.569	1.00	37.62
	ATOM	1976	CB	LEU	B	310	17.205	15.969	31.499	1.00	38.84
	ATOM	1977	CG	LEU	B	310	16.216	15.873	32.668	1.00	42.43
	ATOM	1978	CD1	LEU	B	310	16.040	17.219	33.355	1.00	42.55
	ATOM	1979	CD2	LEU	B	310	14.881	15.380	32.138	1.00	39.69
	ATOM	1980	C	LEU	B	310	19.691	16.174	31.285	1.00	34.11
	ATOM	1981	O	LEU	B	310	20.111	16.070	30.139	1.00	34.41
	ATOM	1982	N	THR	B	311	20.339	15.662	32.326	1.00	34.04
	ATOM	1983	CA	THR	B	311	21.564	14.888	32.127	1.00	32.34
	ATOM	1984	CB	THR	B	311	22.434	14.824	33.399	1.00	31.75
	ATOM	1985	OG1	THR	B	311	21.724	14.116	34.420	1.00	36.20
	ATOM	1986	CG2	THR	B	311	22.782	16.212	33.893	1.00	31.05
	ATOM	1987	C	THR	B	311	21.145	13.460	31.790	1.00	32.37
	ATOM	1988	O	THR	B	311	19.967	13.117	31.899	1.00	28.16
	ATOM	1989	N	ALA	B	312	22.106	12.628	31.396	1.00	33.23
	ATOM	1990	CA	ALA	B	312	21.811	11.237	31.053	1.00	35.63
	ATOM	1991	CB	ALA	B	312	23.077	10.527	30.577	1.00	34.00
	ATOM	1992	C	ALA	B	312	21.210	10.489	32.240	1.00	34.29
	ATOM	1993	O	ALA	B	312	20.226	9.766	32.089	1.00	33.10
	ATOM	1994	N	ASP	B	313	21.800	10.665	33.419	1.00	33.90
	ATOM	1995	CA	ASP	B	313	21.304	9.994	34.615	1.00	34.19
	ATOM	1996	CB	ASP	B	313	22.258	10.219	35.788	1.00	42.09
	ATOM	1997	CG	ASP	B	313	23.494	9.358	35.700	1.00	44.87
	ATOM	1998	OD1	ASP	B	313	24.586	9.858	36.040	1.00	51.57
	ATOM	1999	OD2	ASP	B	313	23.377	8.184	35.290	1.00	46.79
	ATOM	2000	C	ASP	B	313	19.925	10.520	34.971	1.00	31.99
	ATOM	2001	O	ASP	B	313	19.056	9.768	35.426	1.00	32.03
	ATOM	2002	N	GLN	B	314	19.733	11.819	34.763	1.00	29.38
	ATOM	2003	CA	GLN	B	314	18.458	12.457	35.046	1.00	29.73

ATOM	2004	CB	GLN	B	314	18.562	13.966	34.832	1.00	32.88
ATOM	2005	CG	GLN	B	314	18.970	14.732	36.085	1.00	36.47
ATOM	2006	CD	GLN	B	314	19.213	16.208	35.815	1.00	36.76
ATOM	2007	OE1	GLN	B	314	19.300	16.634	34.664	1.00	38.79
ATOM	2008	NE2	GLN	B	314	19.327	16.995	36.880	1.00	39.72
ATOM	2009	C	GLN	B	314	17.409	11.873	34.116	1.00	29.11
ATOM	2010	O	GLN	B	314	16.274	11.620	34.522	1.00	28.82
ATOM	2011	N	MET	B	315	17.801	11.657	32.864	1.00	27.27
ATOM	2012	CA	MET	B	315	16.900	11.079	31.872	1.00	30.41
ATOM	2013	CB	MET	B	315	17.595	11.029	30.509	1.00	30.10
ATOM	2014	CG	MET	B	315	16.787	10.345	29.421	1.00	38.02
ATOM	2015	SD	MET	B	315	15.252	11.220	29.065	1.00	41.12
ATOM	2016	CE	MET	B	315	15.890	12.835	28.611	1.00	39.32
ATOM	2017	C	MET	B	315	16.490	9.665	32.311	1.00	27.99
ATOM	2018	O	MET	B	315	15.302	9.351	32.396	1.00	26.60
ATOM	2019	N	VAL	B	316	17.481	8.823	32.598	1.00	27.26
ATOM	2020	CA	VAL	B	316	17.229	7.447	33.027	1.00	24.54
ATOM	2021	CB	VAL	B	316	18.554	6.708	33.351	1.00	26.22
ATOM	2022	CG1	VAL	B	316	18.272	5.404	34.096	1.00	29.81
ATOM	2023	CG2	VAL	B	316	19.302	6.410	32.074	1.00	29.75
ATOM	2024	C	VAL	B	316	16.326	7.389	34.258	1.00	27.22
ATOM	2025	O	VAL	B	316	15.397	6.579	34.318	1.00	25.55
ATOM	2026	N	SER	B	317	16.601	8.243	35.242	1.00	24.40
ATOM	2027	CA	SER	B	317	15.799	8.268	36.460	1.00	27.63
ATOM	2028	CB	SER	B	317	16.358	9.294	37.451	1.00	31.68
ATOM	2029	OG	SER	B	317	17.492	8.771	38.112	1.00	39.97
ATOM	2030	C	SER	B	317	14.346	8.600	36.154	1.00	26.73
ATOM	2031	O	SER	B	317	13.434	7.932	36.648	1.00	25.65
ATOM	2032	N	ALA	B	318	14.135	9.634	35.342	1.00	24.19
ATOM	2033	CA	ALA	B	318	12.786	10.049	34.969	1.00	24.17
ATOM	2034	CB	ALA	B	318	12.850	11.250	34.022	1.00	21.44
ATOM	2035	C	ALA	B	318	12.038	8.890	34.306	1.00	21.63
ATOM	2036	O	ALA	B	318	10.902	8.598	34.648	1.00	20.25
ATOM	2037	N	LEU	B	319	12.695	8.225	33.364	1.00	23.37
ATOM	2038	CA	LEU	B	319	12.098	7.102	32.652	1.00	25.42
ATOM	2039	CB	LEU	B	319	13.050	6.635	31.548	1.00	22.03
ATOM	2040	CG	LEU	B	319	13.264	7.622	30.394	1.00	20.71
ATOM	2041	CD1	LEU	B	319	14.146	6.995	29.331	1.00	23.60
ATOM	2042	CD2	LEU	B	319	11.918	8.020	29.803	1.00	23.82
ATOM	2043	C	LEU	B	319	11.729	5.926	33.564	1.00	27.26
ATOM	2044	O	LEU	B	319	10.615	5.396	33.488	1.00	28.91
ATOM	2045	N	LEU	B	320	12.656	5.516	34.426	1.00	26.58
ATOM	2046	CA	LEU	B	320	12.399	4.405	35.334	1.00	26.73
ATOM	2047	CB	LEU	B	320	13.657	4.075	36.145	1.00	26.87
ATOM	2048	CG	LEU	B	320	14.846	3.460	35.398	1.00	26.15
ATOM	2049	CD1	LEU	B	320	16.053	3.375	36.330	1.00	28.04
ATOM	2050	CD2	LEU	B	320	14.484	2.076	34.895	1.00	26.96
ATOM	2051	C	LEU	B	320	11.249	4.722	36.290	1.00	29.19

ATOM	2052	O	LEU	B	320	10.449	3.849	36.631	1.00	26.66
ATOM	2053	N	ASP	B	321	11.160	5.976	36.719	1.00	29.72
ATOM	2054	CA	ASP	B	321	10.112	6.371	37.647	1.00	31.36
ATOM	2055	CB	ASP	B	321	10.494	7.683	38.336	1.00	36.60
ATOM	2056	CG	ASP	B	321	11.407	7.461	39.535	1.00	46.11
ATOM	2057	OD1	ASP	B	321	10.897	7.058	40.605	1.00	46.64
ATOM	2058	OD2	ASP	B	321	12.635	7.676	39.402	1.00	45.98
ATOM	2059	C	ASP	B	321	8.742	6.494	36.989	1.00	28.29
ATOM	2060	O	ASP	B	321	7.715	6.432	37.661	1.00	27.19
ATOM	2061	N	ALA	B	322	8.726	6.650	35.672	1.00	28.34
ATOM	2062	CA	ALA	B	322	7.469	6.779	34.950	1.00	25.55
ATOM	2063	CB	ALA	B	322	7.668	7.668	33.728	1.00	24.11
ATOM	2064	C	ALA	B	322	6.911	5.420	34.523	1.00	22.80
ATOM	2065	O	ALA	B	322	5.810	5.338	33.979	1.00	24.54
ATOM	2066	N	GLU	B	323	7.662	4.355	34.781	1.00	20.16
ATOM	2067	CA	GLU	B	323	7.229	3.021	34.386	1.00	21.44
ATOM	2068	CB	GLU	B	323	8.196	1.982	34.938	1.00	23.72
ATOM	2069	CG	GLU	B	323	9.393	1.746	34.024	1.00	23.58
ATOM	2070	CD	GLU	B	323	8.988	1.134	32.685	1.00	25.23
ATOM	2071	OE1	GLU	B	323	8.852	1.881	31.692	1.00	21.74
ATOM	2072	OE2	GLU	B	323	8.809	-0.095	32.624	1.00	25.49
ATOM	2073	C	GLU	B	323	5.796	2.696	34.810	1.00	22.35
ATOM	2074	O	GLU	B	323	5.409	2.926	35.951	1.00	22.34
ATOM	2075	N	PRO	B	324	4.986	2.165	33.880	1.00	19.10
ATOM	2076	CD	PRO	B	324	5.286	1.806	32.483	1.00	19.11
ATOM	2077	CA	PRO	B	324	3.607	1.839	34.242	1.00	22.04
ATOM	2078	CB	PRO	B	324	2.919	1.658	32.893	1.00	21.96
ATOM	2079	CG	PRO	B	324	4.015	1.137	32.015	1.00	24.13
ATOM	2080	C	PRO	B	324	3.619	0.556	35.060	1.00	23.44
ATOM	2081	O	PRO	B	324	4.590	-0.200	35.028	1.00	22.20
ATOM	2082	N	PRO	B	325	2.540	0.287	35.801	1.00	24.88
ATOM	2083	CD	PRO	B	325	1.299	1.068	35.945	1.00	26.67
ATOM	2084	CA	PRO	B	325	2.520	-0.940	36.603	1.00	25.10
ATOM	2085	CB	PRO	B	325	1.394	-0.691	37.595	1.00	27.09
ATOM	2086	CG	PRO	B	325	0.448	0.205	36.854	1.00	26.87
ATOM	2087	C	PRO	B	325	2.270	-2.192	35.776	1.00	25.77
ATOM	2088	O	PRO	B	325	1.853	-2.118	34.617	1.00	21.69
ATOM	2089	N	ILE	B	326	2.538	-3.344	36.379	1.00	24.05
ATOM	2090	CA	ILE	B	326	2.301	-4.620	35.722	1.00	22.51
ATOM	2091	CB	ILE	B	326	3.303	-5.688	36.185	1.00	25.81
ATOM	2092	CG2	ILE	B	326	3.011	-7.018	35.481	1.00	23.78
ATOM	2093	CG1	ILE	B	326	4.729	-5.209	35.900	1.00	25.75
ATOM	2094	CD1	ILE	B	326	5.241	-5.585	34.533	1.00	27.78
ATOM	2095	C	ILE	B	326	0.893	-5.020	36.149	1.00	23.63
ATOM	2096	O	ILE	B	326	0.632	-5.231	37.332	1.00	24.81
ATOM	2097	N	LEU	B	327	-0.018	-5.104	35.188	1.00	19.44
ATOM	2098	CA	LEU	B	327	-1.399	-5.437	35.493	1.00	17.03
ATOM	2099	CB	LEU	B	327	-2.336	-4.747	34.493	1.00	18.39

ATOM	2100	CG	LEU	B	327	-2.201	-3.216	34.373	1.00	20.69
ATOM	2101	CD1	LEU	B	327	-3.245	-2.679	33.406	1.00	14.87
ATOM	2102	CD2	LEU	B	327	-2.384	-2.570	35.742	1.00	14.39
ATOM	2103	C	LEU	B	327	-1.662	-6.928	35.499	1.00	19.87
ATOM	2104	O	LEU	B	327	-0.854	-7.722	35.014	1.00	20.90
ATOM	2105	N	TYR	B	328	-2.803	-7.300	36.066	1.00	20.92
ATOM	2106	CA	TYR	B	328	-3.202	-8.692	36.135	1.00	21.79
ATOM	2107	CB	TYR	B	328	-3.658	-9.050	37.550	1.00	22.91
ATOM	2108	CG	TYR	B	328	-2.515	-9.376	38.468	1.00	24.60
ATOM	2109	CD1	TYR	B	328	-2.118	-10.696	38.677	1.00	25.93
ATOM	2110	CE1	TYR	B	328	-1.034	-11.000	39.498	1.00	28.10
ATOM	2111	CD2	TYR	B	328	-1.802	-8.362	39.103	1.00	29.46
ATOM	2112	CE2	TYR	B	328	-0.716	-8.654	39.926	1.00	35.30
ATOM	2113	CZ	TYR	B	328	-0.338	-9.973	40.117	1.00	32.59
ATOM	2114	OH	TYR	B	328	0.739	-10.257	40.923	1.00	37.24
ATOM	2115	C	TYR	B	328	-4.336	-8.944	35.168	1.00	22.25
ATOM	2116	O	TYR	B	328	-5.115	-8.039	34.849	1.00	19.77
ATOM	2117	N	SER	B	329	-4.420	-10.180	34.698	1.00	25.81
ATOM	2118	CA	SER	B	329	-5.480	-10.571	33.787	1.00	29.39
ATOM	2119	CB	SER	B	329	-5.002	-11.710	32.887	1.00	27.65
ATOM	2120	OG	SER	B	329	-6.091	-12.329	32.233	1.00	28.98
ATOM	2121	C	SER	B	329	-6.625	-11.042	34.673	1.00	33.17
ATOM	2122	O	SER	B	329	-6.453	-11.157	35.888	1.00	32.52
ATOM	2123	N	GLU	B	330	-7.792	-11.289	34.084	1.00	38.75
ATOM	2124	CA	GLU	B	330	-8.930	-11.776	34.859	1.00	44.91
ATOM	2125	CB	GLU	B	330	-10.134	-11.999	33.951	1.00	45.63
ATOM	2126	C	GLU	B	330	-8.493	-13.093	35.491	1.00	48.62
ATOM	2127	O	GLU	B	330	-7.739	-13.851	34.882	1.00	52.37
ATOM	2128	N	TYR	B	331	-8.952	-13.366	36.707	1.00	51.75
ATOM	2129	CA	TYR	B	331	-8.575	-14.596	37.396	1.00	55.25
ATOM	2130	CB	TYR	B	331	-8.538	-14.365	38.911	1.00	53.04
ATOM	2131	CG	TYR	B	331	-9.769	-13.668	39.440	1.00	50.70
ATOM	2132	CD1	TYR	B	331	-10.880	-14.400	39.856	1.00	47.09
ATOM	2133	CE1	TYR	B	331	-12.035	-13.762	40.292	1.00	46.43
ATOM	2134	CD2	TYR	B	331	-9.842	-12.273	39.478	1.00	47.52
ATOM	2135	CE2	TYR	B	331	-10.993	-11.625	39.913	1.00	43.98
ATOM	2136	CZ	TYR	B	331	-12.086	-12.376	40.314	1.00	44.33
ATOM	2137	OH	TYR	B	331	-13.239	-11.747	40.715	1.00	45.31
ATOM	2138	C	TYR	B	331	-9.528	-15.743	37.075	1.00	60.11
ATOM	2139	O	TYR	B	331	-10.748	-15.569	37.066	1.00	63.13
ATOM	2140	N	ASP	B	332	-8.952	-16.913	36.809	1.00	61.60
ATOM	2141	CA	ASP	B	332	-9.704	-18.124	36.490	1.00	63.58
ATOM	2142	CB	ASP	B	332	-10.637	-17.895	35.298	1.00	65.11
ATOM	2143	CG	ASP	B	332	-11.723	-18.953	35.200	1.00	65.32
ATOM	2144	OD1	ASP	B	332	-11.420	-20.136	35.463	1.00	63.69
ATOM	2145	OD2	ASP	B	332	-12.876	-18.602	34.866	1.00	63.61
ATOM	2146	C	ASP	B	332	-8.707	-19.227	36.153	1.00	62.86
ATOM	2147	O	ASP	B	332	-7.853	-19.056	35.287	1.00	62.26

	ATOM	2148	N	PRO	B	333	-8.811	-20.379	36.833	1.00	63.96
	ATOM	2149	CD	PRO	B	333	-9.808	-20.690	37.875	1.00	64.24
	ATOM	2150	CA	PRO	B	333	-7.901	-21.503	36.596	1.00	64.24
	ATOM	2151	CB	PRO	B	333	-8.015	-22.325	37.874	1.00	64.70
	ATOM	2152	CG	PRO	B	333	-9.410	-22.071	38.347	1.00	65.00
	ATOM	2153	C	PRO	B	333	-8.180	-22.340	35.351	1.00	63.90
	ATOM	2154	O	PRO	B	333	-7.384	-23.214	35.007	1.00	63.70
	ATOM	2155	N	THR	B	334	-9.303	-22.084	34.683	1.00	63.83
	ATOM	2156	CA	THR	B	334	-9.649	-22.832	33.475	1.00	63.77
	ATOM	2157	CB	THR	B	334	-11.065	-22.477	32.975	1.00	64.63
	ATOM	2158	OG1	THR	B	334	-11.132	-21.078	32.675	1.00	65.95
	ATOM	2159	CG2	THR	B	334	-12.102	-22.817	34.036	1.00	65.09
	ATOM	2160	C	THR	B	334	-8.634	-22.499	32.388	1.00	62.62
	ATOM	2161	O	THR	B	334	-8.931	-21.774	31.437	1.00	60.15
	ATOM	2162	N	ARG	B	335	-7.432	-23.043	32.553	1.00	63.14
	ATOM	2163	CA	ARG	B	335	-6.324	-22.820	31.633	1.00	60.70
	ATOM	2164	CB	ARG	B	335	-5.130	-23.667	32.050	1.00	58.73
	ATOM	2165	C	ARG	B	335	-6.667	-23.086	30.174	1.00	59.71
	ATOM	2166	O	ARG	B	335	-6.302	-22.298	29.298	1.00	62.33
	ATOM	2167	N	PRO	B	336	-7.377	-24.194	29.884	1.00	55.25
	ATOM	2168	CD	PRO	B	336	-7.938	-25.227	30.769	1.00	53.53
	ATOM	2169	CA	PRO	B	336	-7.698	-24.437	28.471	1.00	50.10
	ATOM	2170	CB	PRO	B	336	-8.399	-25.799	28.476	1.00	49.70
	ATOM	2171	CG	PRO	B	336	-8.164	-26.372	29.844	1.00	50.71
	ATOM	2172	C	PRO	B	336	-8.602	-23.324	27.954	1.00	44.54
	ATOM	2173	O	PRO	B	336	-9.809	-23.342	28.179	1.00	44.14
	ATOM	2174	N	PHE	B	337	-8.007	-22.350	27.274	1.00	39.18
	ATOM	2175	CA	PHE	B	337	-8.764	-21.223	26.742	1.00	38.25
	ATOM	2176	CB	PHE	B	337	-7.850	-20.003	26.567	1.00	36.98
	ATOM	2177	CG	PHE	B	337	-7.229	-19.517	27.846	1.00	36.81
	ATOM	2178	CD1	PHE	B	337	-5.846	-19.511	28.002	1.00	38.89
	ATOM	2179	CD2	PHE	B	337	-8.023	-19.062	28.893	1.00	35.97
	ATOM	2180	CE1	PHE	B	337	-5.262	-19.059	29.185	1.00	36.85
	ATOM	2181	CE2	PHE	B	337	-7.449	-18.608	30.079	1.00	37.15
	ATOM	2182	CZ	PHE	B	337	-6.064	-18.607	30.224	1.00	38.40
	ATOM	2183	C	PHE	B	337	-9.420	-21.535	25.402	1.00	36.81
	ATOM	2184	O	PHE	B	337	-8.962	-22.399	24.658	1.00	36.26
	ATOM	2185	N	SER	B	338	-10.504	-20.828	25.107	1.00	35.85
	ATOM	2186	CA	SER	B	338	-11.198	-20.981	23.836	1.00	34.76
	ATOM	2187	CB	SER	B	338	-12.713	-20.948	24.035	1.00	34.85
	ATOM	2188	OG	SER	B	338	-13.164	-19.621	24.235	1.00	33.53
	ATOM	2189	C	SER	B	338	-10.761	-19.761	23.037	1.00	34.99
	ATOM	2190	O	SER	B	338	-10.143	-18.855	23.591	1.00	34.32
	ATOM	2191	N	GLU	B	339	-11.075	-19.722	21.750	1.00	33.01
	ATOM	2192	CA	GLU	B	339	-10.682	-18.579	20.950	1.00	33.94
	ATOM	2193	CB	GLU	B	339	-11.146	-18.737	19.501	1.00	33.79
	ATOM	2194	CG	GLU	B	339	-10.758	-17.553	18.623	1.00	39.11
	ATOM	2195	CD	GLU	B	339	-10.865	-17.852	17.137	1.00	43.17

ATOM	2196	OE1	GLU	B	339	-11.990	-17.785	16.600	1.00	45.28
ATOM	2197	OE2	GLU	B	339	-9.824	-18.152	16.510	1.00	39.19
ATOM	2198	C	GLU	B	339	-11.265	-17.295	21.531	1.00	34.28
ATOM	2199	O	GLU	B	339	-10.575	-16.283	21.631	1.00	33.65
ATOM	2200	N	ALA	B	340	-12.535	-17.339	21.920	1.00	31.12
ATOM	2201	CA	ALA	B	340	-13.194	-16.164	22.469	1.00	29.10
ATOM	2202	CB	ALA	B	340	-14.696	-16.412	22.573	1.00	33.84
ATOM	2203	C	ALA	B	340	-12.639	-15.731	23.826	1.00	28.98
ATOM	2204	O	ALA	B	340	-12.431	-14.541	24.060	1.00	30.48
ATOM	2205	N	SER	B	341	-12.407	-16.691	24.719	1.00	26.66
ATOM	2206	CA	SER	B	341	-11.882	-16.386	26.044	1.00	24.26
ATOM	2207	CB	SER	B	341	-11.867	-17.643	26.923	1.00	27.04
ATOM	2208	OG	SER	B	341	-10.851	-18.541	26.515	1.00	33.84
ATOM	2209	C	SER	B	341	-10.479	-15.793	25.960	1.00	23.97
ATOM	2210	O	SER	B	341	-10.171	-14.824	26.651	1.00	21.56
ATOM	2211	N	MET	B	342	-9.631	-16.368	25.114	1.00	26.83
ATOM	2212	CA	MET	B	342	-8.271	-15.865	24.954	1.00	27.24
ATOM	2213	CB	MET	B	342	-7.477	-16.758	24.001	1.00	30.45
ATOM	2214	CG	MET	B	342	-6.038	-16.300	23.802	1.00	35.35
ATOM	2215	SD	MET	B	342	-4.866	-17.667	23.777	1.00	44.57
ATOM	2216	CE	MET	B	342	-4.034	-17.341	22.244	1.00	41.37
ATOM	2217	C	MET	B	342	-8.322	-14.448	24.385	1.00	25.31
ATOM	2218	O	MET	B	342	-7.653	-13.541	24.874	1.00	26.67
ATOM	2219	N	MET	B	343	-9.114	-14.278	23.345	1.00	25.75
ATOM	2220	CA	MET	B	343	-9.262	-12.979	22.712	1.00	25.47
ATOM	2221	CB	MET	B	343	-10.210	-13.088	21.528	1.00	23.51
ATOM	2222	CG	MET	B	343	-9.540	-13.618	20.273	1.00	28.86
ATOM	2223	SD	MET	B	343	-8.325	-12.456	19.609	1.00	29.25
ATOM	2224	CE	MET	B	343	-9.344	-11.015	19.371	1.00	28.74
ATOM	2225	C	MET	B	343	-9.798	-11.966	23.712	1.00	25.37
ATOM	2226	O	MET	B	343	-9.360	-10.810	23.728	1.00	24.98
ATOM	2227	N	GLY	B	344	-10.739	-12.403	24.536	1.00	23.91
ATOM	2228	CA	GLY	B	344	-11.320	-11.526	25.536	1.00	22.43
ATOM	2229	C	GLY	B	344	-10.313	-11.103	26.592	1.00	22.06
ATOM	2230	O	GLY	B	344	-10.262	-9.934	26.982	1.00	20.87
ATOM	2231	N	LEU	B	345	-9.511	-12.048	27.063	1.00	19.36
ATOM	2232	CA	LEU	B	345	-8.520	-11.748	28.083	1.00	25.74
ATOM	2233	CB	LEU	B	345	-7.886	-13.040	28.600	1.00	26.78
ATOM	2234	CG	LEU	B	345	-8.794	-14.010	29.362	1.00	30.04
ATOM	2235	CD1	LEU	B	345	-8.099	-15.357	29.488	1.00	28.39
ATOM	2236	CD2	LEU	B	345	-9.122	-13.443	30.736	1.00	29.93
ATOM	2237	C	LEU	B	345	-7.425	-10.822	27.550	1.00	23.24
ATOM	2238	O	LEU	B	345	-7.037	-9.865	28.212	1.00	23.43
ATOM	2239	N	LEU	B	346	-6.937	-11.108	26.350	1.00	21.92
ATOM	2240	CA	LEU	B	346	-5.874	-10.303	25.763	1.00	22.71
ATOM	2241	CB	LEU	B	346	-5.343	-10.962	24.486	1.00	23.17
ATOM	2242	CG	LEU	B	346	-4.684	-12.331	24.668	1.00	20.66
ATOM	2243	CD1	LEU	B	346	-4.303	-12.916	23.309	1.00	18.75

	ATOM	2244	CD2	LEU	B	346	-3.464	-12.188	25.553	1.00	20.84
	ATOM	2245	C	LEU	B	346	-6.304	-8.873	25.458	1.00	22.99
	ATOM	2246	O	LEU	B	346	-5.540	-7.935	25.695	1.00	22.07
	ATOM	2247	N	THR	B	347	-7.516	-8.699	24.937	1.00	20.53
5	ATOM	2248	CA	THR	B	347	-7.987	-7.357	24.608	1.00	21.89
	ATOM	2249	CB	THR	B	347	-9.152	-7.388	23.601	1.00	21.65
	ATOM	2250	OG1	THR	B	347	-10.218	-8.190	24.123	1.00	19.65
	ATOM	2251	CG2	THR	B	347	-8.676	-7.955	22.262	1.00	22.01
	ATOM	2252	C	THR	B	347	-8.426	-6.590	25.853	1.00	23.60
10	ATOM	2253	O	THR	B	347	-8.358	-5.357	25.883	1.00	20.31
	ATOM	2254	N	ASN	B	348	-8.884	-7.314	26.874	1.00	22.27
	ATOM	2255	CA	ASN	B	348	-9.293	-6.667	28.114	1.00	23.99
	ATOM	2256	CB	ASN	B	348	-10.008	-7.642	29.056	1.00	22.32
	ATOM	2257	CG	ASN	B	348	-10.342	-7.022	30.398	1.00	28.26
15	ATOM	2258	OD1	ASN	B	348	-9.478	-6.746	31.216	1.00	27.14
	ATOM	2259	ND2	ASN	B	348	-11.647	-6.764	30.625	1.00	27.02
	ATOM	2260	C	ASN	B	348	-8.035	-6.120	28.798	1.00	19.48
	ATOM	2261	O	ASN	B	348	-8.014	-4.991	29.271	1.00	18.26
	ATOM	2262	N	LEU	B	349	-6.984	-6.931	28.832	1.00	19.07
20	ATOM	2263	CA	LEU	B	349	-5.724	-6.516	29.446	1.00	20.37
	ATOM	2264	CB	LEU	B	349	-4.716	-7.674	29.434	1.00	18.21
	ATOM	2265	CG	LEU	B	349	-3.297	-7.316	29.889	1.00	18.24
	ATOM	2266	CD1	LEU	B	349	-3.323	-6.904	31.356	1.00	12.44
	ATOM	2267	CD2	LEU	B	349	-2.370	-8.504	29.672	1.00	21.28
25	ATOM	2268	C	LEU	B	349	-5.131	-5.307	28.718	1.00	19.92
	ATOM	2269	O	LEU	B	349	-4.738	-4.322	29.349	1.00	16.56
	ATOM	2270	N	ALA	B	350	-5.067	-5.391	27.391	1.00	16.67
	ATOM	2271	CA	ALA	B	350	-4.529	-4.308	26.578	1.00	17.11
	ATOM	2272	CB	ALA	B	350	-4.587	-4.690	25.095	1.00	14.15
30	ATOM	2273	C	ALA	B	350	-5.272	-2.988	26.805	1.00	17.92
	ATOM	2274	O	ALA	B	350	-4.650	-1.926	26.904	1.00	18.71
	ATOM	2275	N	ASP	B	351	-6.600	-3.053	26.857	1.00	17.51
	ATOM	2276	CA	ASP	B	351	-7.409	-1.856	27.074	1.00	16.57
	ATOM	2277	CB	ASP	B	351	-8.902	-2.202	27.041	1.00	18.97
35	ATOM	2278	CG	ASP	B	351	-9.785	-0.974	26.858	1.00	21.80
	ATOM	2279	OD1	ASP	B	351	-9.660	-0.292	25.824	1.00	24.62
	ATOM	2280	OD2	ASP	B	351	-10.604	-0.682	27.754	1.00	22.78
	ATOM	2281	C	ASP	B	351	-7.064	-1.228	28.415	1.00	16.81
	ATOM	2282	O	ASP	B	351	-6.963	-0.009	28.534	1.00	15.75
40	ATOM	2283	N	ARG	B	352	-6.894	-2.056	29.438	1.00	13.97
	ATOM	2284	CA	ARG	B	352	-6.552	-1.509	30.742	1.00	16.09
	ATOM	2285	CB	ARG	B	352	-6.728	-2.571	31.833	1.00	15.78
	ATOM	2286	CG	ARG	B	352	-8.189	-2.819	32.189	1.00	17.93
	ATOM	2287	CD	ARG	B	352	-8.323	-3.882	33.279	1.00	19.84
45	ATOM	2288	NE	ARG	B	352	-8.010	-5.222	32.785	1.00	21.36
	ATOM	2289	CZ	ARG	B	352	-7.187	-6.075	33.387	1.00	21.18
	ATOM	2290	NH1	ARG	B	352	-6.579	-5.741	34.516	1.00	20.51
	ATOM	2291	NH2	ARG	B	352	-6.980	-7.275	32.864	1.00	28.51

ATOM	2292	C	ARG	B	352	-5.123	-0.975	30.728	1.00	15.81
ATOM	2293	O	ARG	B	352	-4.835	0.057	31.339	1.00	15.61
ATOM	2294	N	GLU	B	353	-4.231	-1.665	30.019	1.00	15.45
ATOM	2295	CA	GLU	B	353	-2.838	-1.228	29.935	1.00	16.59
ATOM	2296	CB	GLU	B	353	-1.990	-2.243	29.168	1.00	14.64
ATOM	2297	CG	GLU	B	353	-1.554	-3.456	29.973	1.00	18.23
ATOM	2298	CD	GLU	B	353	-0.620	-4.355	29.176	1.00	22.72
ATOM	2299	OE1	GLU	B	353	-1.099	-5.078	28.275	1.00	21.94
ATOM	2300	OE2	GLU	B	353	0.599	-4.324	29.442	1.00	24.41
ATOM	2301	C	GLU	B	353	-2.729	0.119	29.219	1.00	15.85
ATOM	2302	O	GLU	B	353	-1.872	0.939	29.540	1.00	13.76
ATOM	2303	N	LEU	B	354	-3.594	0.335	28.235	1.00	12.93
ATOM	2304	CA	LEU	B	354	-3.556	1.575	27.472	1.00	15.33
ATOM	2305	CB	LEU	B	354	-4.616	1.534	26.360	1.00	16.44
ATOM	2306	CG	LEU	B	354	-4.174	0.750	25.112	1.00	17.03
ATOM	2307	CD1	LEU	B	354	-5.373	0.509	24.189	1.00	16.70
ATOM	2308	CD2	LEU	B	354	-3.069	1.531	24.384	1.00	14.52
ATOM	2309	C	LEU	B	354	-3.747	2.805	28.361	1.00	12.78
ATOM	2310	O	LEU	B	354	-3.123	3.850	28.141	1.00	14.28
ATOM	2311	N	VAL	B	355	-4.600	2.682	29.369	1.00	12.60
ATOM	2312	CA	VAL	B	355	-4.844	3.791	30.279	1.00	16.78
ATOM	2313	CB	VAL	B	355	-5.925	3.429	31.327	1.00	16.84
ATOM	2314	CG1	VAL	B	355	-6.070	4.561	32.344	1.00	19.88
ATOM	2315	CG2	VAL	B	355	-7.254	3.187	30.639	1.00	19.33
ATOM	2316	C	VAL	B	355	-3.533	4.161	30.986	1.00	19.17
ATOM	2317	O	VAL	B	355	-3.158	5.328	31.049	1.00	17.30
ATOM	2318	N	HIS	B	356	-2.826	3.160	31.499	1.00	19.68
ATOM	2319	CA	HIS	B	356	-1.559	3.418	32.177	1.00	20.64
ATOM	2320	CB	HIS	B	356	-1.110	2.174	32.945	1.00	21.03
ATOM	2321	CG	HIS	B	356	-2.018	1.818	34.085	1.00	22.88
ATOM	2322	CD2	HIS	B	356	-3.128	1.045	34.135	1.00	21.70
ATOM	2323	ND1	HIS	B	356	-1.838	2.312	35.358	1.00	19.24
ATOM	2324	CE1	HIS	B	356	-2.802	1.860	36.145	1.00	18.84
ATOM	2325	NE2	HIS	B	356	-3.598	1.088	35.426	1.00	17.92
ATOM	2326	C	HIS	B	356	-0.479	3.861	31.184	1.00	19.67
ATOM	2327	O	HIS	B	356	0.424	4.614	31.547	1.00	19.61
ATOM	2328	N	MET	B	357	-0.566	3.413	29.931	1.00	14.92
ATOM	2329	CA	MET	B	357	0.428	3.830	28.939	1.00	15.13
ATOM	2330	CB	MET	B	357	0.239	3.099	27.604	1.00	13.94
ATOM	2331	CG	MET	B	357	1.149	3.631	26.476	1.00	14.71
ATOM	2332	SD	MET	B	357	0.747	3.014	24.826	1.00	17.75
ATOM	2333	CE	MET	B	357	0.746	1.222	25.122	1.00	15.21
ATOM	2334	C	MET	B	357	0.316	5.334	28.699	1.00	14.94
ATOM	2335	O	MET	B	357	1.319	6.031	28.560	1.00	17.02
ATOM	2336	N	ILE	B	358	-0.909	5.839	28.659	1.00	18.01
ATOM	2337	CA	ILE	B	358	-1.122	7.263	28.423	1.00	19.77
ATOM	2338	CB	ILE	B	358	-2.634	7.577	28.287	1.00	23.11
ATOM	2339	CG2	ILE	B	358	-2.879	9.080	28.450	1.00	25.00

	ATOM	2340	CG1	ILE	B	358	-3.137	7.105	26.913	1.00	24.19
	ATOM	2341	CD1	ILE	B	358	-4.600	6.653	26.890	1.00	20.17
	ATOM	2342	C	ILE	B	358	-0.501	8.100	29.550	1.00	22.93
	ATOM	2343	O	ILE	B	358	0.080	9.153	29.299	1.00	23.33
	ATOM	2344	N	ASN	B	359	-0.619	7.631	30.790	1.00	22.34
	ATOM	2345	CA	ASN	B	359	-0.029	8.341	31.924	1.00	23.24
	ATOM	2346	CB	ASN	B	359	-0.480	7.726	33.224	1.00	25.10
	ATOM	2347	CG	ASN	B	359	-1.831	8.171	33.649	1.00	32.65
	ATOM	2348	OD1	ASN	B	359	-2.421	9.069	33.042	1.00	32.98
	ATOM	2349	ND2	ASN	B	359	-2.364	7.549	34.691	1.00	33.87
	ATOM	2350	C	ASN	B	359	1.473	8.306	31.837	1.00	24.77
	ATOM	2351	O	ASN	B	359	2.152	9.285	32.149	1.00	24.19
	ATOM	2352	N	TRP	B	360	1.995	7.149	31.438	1.00	20.82
	ATOM	2353	CA	TRP	B	360	3.439	6.965	31.310	1.00	19.29
	ATOM	2354	CB	TRP	B	360	3.754	5.524	30.878	1.00	18.59
	ATOM	2355	CG	TRP	B	360	5.085	5.363	30.176	1.00	18.21
	ATOM	2356	CD2	TRP	B	360	5.310	5.308	28.756	1.00	14.38
	ATOM	2357	CE2	TRP	B	360	6.698	5.129	28.561	1.00	13.42
	ATOM	2358	CE3	TRP	B	360	4.475	5.392	27.633	1.00	15.52
	ATOM	2359	CD1	TRP	B	360	6.306	5.221	30.762	1.00	13.34
	ATOM	2360	NE1	TRP	B	360	7.283	5.078	29.800	1.00	16.05
	ATOM	2361	CZ2	TRP	B	360	7.272	5.032	27.288	1.00	16.84
	ATOM	2362	CZ3	TRP	B	360	5.045	5.296	26.363	1.00	15.11
	ATOM	2363	CH2	TRP	B	360	6.431	5.115	26.202	1.00	16.12
	ATOM	2364	C	TRP	B	360	3.979	7.939	30.273	1.00	20.13
	ATOM	2365	O	TRP	B	360	4.991	8.606	30.497	1.00	17.26
	ATOM	2366	N	ALA	B	361	3.295	8.012	29.135	1.00	19.34
	ATOM	2367	CA	ALA	B	361	3.708	8.900	28.051	1.00	22.01
	ATOM	2368	CB	ALA	B	361	2.682	8.855	26.921	1.00	19.53
	ATOM	2369	C	ALA	B	361	3.883	10.336	28.552	1.00	22.39
	ATOM	2370	O	ALA	B	361	4.858	11.005	28.210	1.00	19.57
	ATOM	2371	N	LYS	B	362	2.932	10.794	29.361	1.00	21.96
	ATOM	2372	CA	LYS	B	362	2.966	12.139	29.923	1.00	26.45
	ATOM	2373	CB	LYS	B	362	1.741	12.363	30.811	1.00	29.79
	ATOM	2374	CG	LYS	B	362	0.426	12.417	30.064	1.00	33.57
	ATOM	2375	CD	LYS	B	362	-0.563	13.304	30.805	1.00	36.83
	ATOM	2376	CE	LYS	B	362	-1.620	12.490	31.512	1.00	36.89
	ATOM	2377	NZ	LYS	B	362	-2.873	13.276	31.664	1.00	39.07
	ATOM	2378	C	LYS	B	362	4.223	12.379	30.757	1.00	27.77
	ATOM	2379	O	LYS	B	362	4.661	13.517	30.922	1.00	26.93
	ATOM	2380	N	ARG	B	363	4.805	11.302	31.278	1.00	26.61
	ATOM	2381	CA	ARG	B	363	5.996	11.414	32.109	1.00	27.74
	ATOM	2382	CB	ARG	B	363	5.887	10.457	33.298	1.00	28.93
	ATOM	2383	CG	ARG	B	363	4.650	10.704	34.158	1.00	36.07
	ATOM	2384	CD	ARG	B	363	4.569	9.745	35.344	1.00	42.83
	ATOM	2385	NE	ARG	B	363	4.477	8.344	34.928	1.00	49.79
	ATOM	2386	CZ	ARG	B	363	3.395	7.582	35.080	1.00	51.48
	ATOM	2387	NH1	ARG	B	363	2.300	8.081	35.648	1.00	52.17

	ATOM	2388	NH2	ARG	B	363	3.405	6.316	34.668	1.00	40.24
	ATOM	2389	C	ARG	B	363	7.308	11.190	31.367	1.00	25.80
	ATOM	2390	O	ARG	B	363	8.374	11.183	31.975	1.00	29.36
	ATOM	2391	N	VAL	B	364	7.231	11.009	30.053	1.00	24.28
5	ATOM	2392	CA	VAL	B	364	8.431	10.823	29.248	1.00	21.87
	ATOM	2393	CB	VAL	B	364	8.116	10.048	27.947	1.00	21.84
	ATOM	2394	CG1	VAL	B	364	9.267	10.184	26.968	1.00	15.85
	ATOM	2395	CG2	VAL	B	364	7.860	8.560	28.268	1.00	16.24
	ATOM	2396	C	VAL	B	364	8.925	12.241	28.923	1.00	28.14
10	ATOM	2397	O	VAL	B	364	8.219	13.023	28.285	1.00	24.24
	ATOM	2398	N	PRO	B	365	10.141	12.591	29.375	1.00	28.57
	ATOM	2399	CD	PRO	B	365	11.061	11.726	30.137	1.00	30.58
	ATOM	2400	CA	PRO	B	365	10.719	13.919	29.138	1.00	32.16
	ATOM	2401	CB	PRO	B	365	12.189	13.739	29.507	1.00	32.70
15	ATOM	2402	CG	PRO	B	365	12.170	12.671	30.545	1.00	33.35
	ATOM	2403	C	PRO	B	365	10.546	14.464	27.726	1.00	32.22
	ATOM	2404	O	PRO	B	365	11.056	13.897	26.766	1.00	37.04
	ATOM	2405	N	GLY	B	366	9.821	15.570	27.609	1.00	34.09
	ATOM	2406	CA	GLY	B	366	9.612	16.182	26.310	1.00	32.54
20	ATOM	2407	C	GLY	B	366	8.241	15.969	25.700	1.00	33.46
	ATOM	2408	O	GLY	B	366	7.791	16.779	24.886	1.00	33.73
	ATOM	2409	N	PHE	B	367	7.564	14.895	26.096	1.00	31.08
	ATOM	2410	CA	PHE	B	367	6.250	14.593	25.542	1.00	28.60
	ATOM	2411	CB	PHE	B	367	5.745	13.244	26.058	1.00	25.96
25	ATOM	2412	CG	PHE	B	367	4.629	12.671	25.239	1.00	22.75
	ATOM	2413	CD1	PHE	B	367	3.313	12.771	25.669	1.00	22.62
	ATOM	2414	CD2	PHE	B	367	4.897	12.025	24.033	1.00	22.29
	ATOM	2415	CE1	PHE	B	367	2.272	12.233	24.914	1.00	25.63
	ATOM	2416	CE2	PHE	B	367	3.867	11.486	23.272	1.00	20.82
30	ATOM	2417	CZ	PHE	B	367	2.553	11.588	23.711	1.00	25.50
	ATOM	2418	C	PHE	B	367	5.178	15.646	25.781	1.00	26.79
	ATOM	2419	O	PHE	B	367	4.458	16.001	24.854	1.00	23.37
	ATOM	2420	N	VAL	B	368	5.049	16.143	27.009	1.00	31.26
	ATOM	2421	CA	VAL	B	368	4.020	17.151	27.277	1.00	35.71
35	ATOM	2422	CB	VAL	B	368	3.817	17.412	28.795	1.00	35.98
	ATOM	2423	CG1	VAL	B	368	2.944	16.320	29.392	1.00	37.64
	ATOM	2424	CG2	VAL	B	368	5.157	17.495	29.508	1.00	35.81
	ATOM	2425	C	VAL	B	368	4.328	18.482	26.598	1.00	35.87
	ATOM	2426	O	VAL	B	368	3.450	19.330	26.457	1.00	37.71
40	ATOM	2427	N	ASP	B	369	5.572	18.665	26.175	1.00	35.49
	ATOM	2428	CA	ASP	B	369	5.950	19.904	25.503	1.00	36.54
	ATOM	2429	CB	ASP	B	369	7.466	19.963	25.309	1.00	39.79
	ATOM	2430	CG	ASP	B	369	8.213	20.169	26.615	1.00	44.33
	ATOM	2431	OD1	ASP	B	369	9.409	19.807	26.684	1.00	48.45
45	ATOM	2432	OD2	ASP	B	369	7.604	20.693	27.572	1.00	43.27
	ATOM	2433	C	ASP	B	369	5.248	19.997	24.149	1.00	34.49
	ATOM	2434	O	ASP	B	369	5.131	21.074	23.571	1.00	34.51
	ATOM	2435	N	LEU	B	370	4.776	18.859	23.653	1.00	30.97

ATOM	2436	CA	LEU	B	370	4.086	18.809	22.370	1.00	29.80
ATOM	2437	CB	LEU	B	370	4.145	17.389	21.799	1.00	27.27
ATOM	2438	CG	LEU	B	370	5.522	16.733	21.688	1.00	28.07
ATOM	2439	CD1	LEU	B	370	5.353	15.242	21.400	1.00	30.38
ATOM	2440	CD2	LEU	B	370	6.316	17.396	20.574	1.00	22.82
ATOM	2441	C	LEU	B	370	2.628	19.218	22.521	1.00	28.04
ATOM	2442	O	LEU	B	370	2.066	19.151	23.611	1.00	29.71
ATOM	2443	N	THR	B	371	2.011	19.645	21.425	1.00	28.70
ATOM	2444	CA	THR	B	371	0.602	20.014	21.474	1.00	30.31
ATOM	2445	CB	THR	B	371	0.150	20.690	20.163	1.00	31.96
ATOM	2446	OG1	THR	B	371	0.284	19.763	19.080	1.00	29.49
ATOM	2447	CG2	THR	B	371	0.991	21.930	19.878	1.00	29.98
ATOM	2448	C	THR	B	371	-0.208	18.726	21.666	1.00	30.59
ATOM	2449	O	THR	B	371	0.300	17.624	21.431	1.00	27.10
ATOM	2450	N	LEU	B	372	-1.461	18.863	22.087	1.00	27.65
ATOM	2451	CA	LEU	B	372	-2.323	17.702	22.303	1.00	30.86
ATOM	2452	CB	LEU	B	372	-3.722	18.147	22.737	1.00	30.11
ATOM	2453	CG	LEU	B	372	-4.715	17.006	22.960	1.00	32.80
ATOM	2454	CD1	LEU	B	372	-4.231	16.147	24.126	1.00	34.10
ATOM	2455	CD2	LEU	B	372	-6.105	17.562	23.246	1.00	31.16
ATOM	2456	C	LEU	B	372	-2.437	16.863	21.034	1.00	31.77
ATOM	2457	O	LEU	B	372	-2.417	15.629	21.078	1.00	27.06
ATOM	2458	N	HIS	B	373	-2.564	17.548	19.905	1.00	31.30
ATOM	2459	CA	HIS	B	373	-2.685	16.888	18.614	1.00	31.35
ATOM	2460	CB	HIS	B	373	-2.844	17.935	17.503	1.00	34.30
ATOM	2461	CG	HIS	B	373	-2.503	17.430	16.132	1.00	41.27
ATOM	2462	CD2	HIS	B	373	-3.293	17.105	15.079	1.00	42.50
ATOM	2463	ND1	HIS	B	373	-1.205	17.220	15.715	1.00	43.69
ATOM	2464	CE1	HIS	B	373	-1.210	16.787	14.465	1.00	48.87
ATOM	2465	NE2	HIS	B	373	-2.465	16.708	14.056	1.00	43.72
ATOM	2466	C	HIS	B	373	-1.468	16.012	18.337	1.00	28.29
ATOM	2467	O	HIS	B	373	-1.610	14.878	17.897	1.00	30.21
ATOM	2468	N	ASP	B	374	-0.275	16.541	18.589	1.00	28.85
ATOM	2469	CA	ASP	B	374	0.950	15.783	18.350	1.00	28.28
ATOM	2470	CB	ASP	B	374	2.178	16.678	18.535	1.00	31.33
ATOM	2471	CG	ASP	B	374	2.433	17.577	17.333	1.00	39.07
ATOM	2472	OD1	ASP	B	374	3.195	18.557	17.478	1.00	40.60
ATOM	2473	OD2	ASP	B	374	1.874	17.305	16.246	1.00	38.64
ATOM	2474	C	ASP	B	374	1.029	14.592	19.303	1.00	29.05
ATOM	2475	O	ASP	B	374	1.432	13.494	18.908	1.00	24.26
ATOM	2476	N	GLN	B	375	0.642	14.814	20.556	1.00	24.52
ATOM	2477	CA	GLN	B	375	0.667	13.749	21.547	1.00	27.37
ATOM	2478	CB	GLN	B	375	0.213	14.270	22.901	1.00	26.66
ATOM	2479	CG	GLN	B	375	1.164	15.236	23.563	1.00	29.74
ATOM	2480	CD	GLN	B	375	0.623	15.691	24.890	1.00	33.13
ATOM	2481	OE1	GLN	B	375	-0.044	14.953	25.602	1.00	32.82
ATOM	2482	NE2	GLN	B	375	0.895	16.953	25.236	1.00	33.98
ATOM	2483	C	GLN	B	375	-0.259	12.630	21.104	1.00	24.52

ATOM	2484	O	GLN	B	375	0.074	11.451	21.221	1.00	23.56
ATOM	2485	N	VAL	B	376	-1.426	13.013	20.599	1.00	21.87
ATOM	2486	CA	VAL	B	376	-2.409	12.055	20.140	1.00	23.44
ATOM	2487	CB	VAL	B	376	-3.718	12.760	19.717	1.00	22.09
ATOM	2488	CG1	VAL	B	376	-4.572	11.823	18.877	1.00	24.14
ATOM	2489	CG2	VAL	B	376	-4.486	13.192	20.954	1.00	16.96
ATOM	2490	C	VAL	B	376	-1.852	11.257	18.965	1.00	24.15
ATOM	2491	O	VAL	B	376	-1.949	10.032	18.938	1.00	22.26
ATOM	2492	N	HIS	B	377	-1.251	11.953	18.007	1.00	25.85
ATOM	2493	CA	HIS	B	377	-0.689	11.284	16.843	1.00	25.68
ATOM	2494	CB	HIS	B	377	-0.078	12.306	15.886	1.00	25.27
ATOM	2495	CG	HIS	B	377	0.535	11.690	14.667	1.00	30.63
ATOM	2496	CD2	HIS	B	377	1.828	11.559	14.287	1.00	31.03
ATOM	2497	ND1	HIS	B	377	-0.217	11.086	13.683	1.00	35.05
ATOM	2498	CE1	HIS	B	377	0.588	10.607	12.750	1.00	33.12
ATOM	2499	NE2	HIS	B	377	1.833	10.882	13.093	1.00	31.06
ATOM	2500	C	HIS	B	377	0.365	10.237	17.210	1.00	24.37
ATOM	2501	O	HIS	B	377	0.321	9.109	16.719	1.00	21.47
ATOM	2502	N	LEU	B	378	1.307	10.609	18.072	1.00	19.24
ATOM	2503	CA	LEU	B	378	2.365	9.691	18.474	1.00	20.09
ATOM	2504	CB	LEU	B	378	3.363	10.402	19.388	1.00	18.64
ATOM	2505	CG	LEU	B	378	4.230	11.489	18.736	1.00	22.15
ATOM	2506	CD1	LEU	B	378	5.104	12.148	19.796	1.00	22.51
ATOM	2507	CD2	LEU	B	378	5.094	10.885	17.638	1.00	20.68
ATOM	2508	C	LEU	B	378	1.832	8.433	19.161	1.00	18.91
ATOM	2509	O	LEU	B	378	2.262	7.320	18.859	1.00	17.52
ATOM	2510	N	LEU	B	379	0.888	8.610	20.077	1.00	18.25
ATOM	2511	CA	LEU	B	379	0.317	7.486	20.795	1.00	18.60
ATOM	2512	CB	LEU	B	379	-0.526	7.989	21.968	1.00	16.77
ATOM	2513	CG	LEU	B	379	0.292	8.353	23.214	1.00	17.90
ATOM	2514	CD1	LEU	B	379	-0.578	9.092	24.211	1.00	15.84
ATOM	2515	CD2	LEU	B	379	0.851	7.075	23.842	1.00	22.09
ATOM	2516	C	LEU	B	379	-0.518	6.605	19.872	1.00	20.17
ATOM	2517	O	LEU	B	379	-0.476	5.377	19.968	1.00	18.11
ATOM	2518	N	GLU	B	380	-1.273	7.222	18.971	1.00	19.40
ATOM	2519	CA	GLU	B	380	-2.086	6.435	18.049	1.00	20.19
ATOM	2520	CB	GLU	B	380	-2.994	7.350	17.222	1.00	22.43
ATOM	2521	CG	GLU	B	380	-4.182	7.874	18.007	1.00	25.30
ATOM	2522	CD	GLU	B	380	-5.070	8.789	17.188	1.00	29.44
ATOM	2523	OE1	GLU	B	380	-6.206	9.066	17.625	1.00	31.70
ATOM	2524	OE2	GLU	B	380	-4.631	9.230	16.110	1.00	31.75
ATOM	2525	C	GLU	B	380	-1.210	5.594	17.117	1.00	18.92
ATOM	2526	O	GLU	B	380	-1.586	4.491	16.722	1.00	19.83
ATOM	2527	N	ACYS	B	381	-0.039	6.113	16.772	0.75	17.41
ATOM	2528	N	BCYS	B	381	-0.035	6.113	16.779	0.25	17.76
ATOM	2529	CA	ACYS	B	381	0.860	5.384	15.887	0.75	20.19
ATOM	2530	CA	BCYS	B	381	0.875	5.407	15.884	0.25	17.50
ATOM	2531	CB	ACYS	B	381	1.870	6.342	15.248	0.75	24.20

ATOM	2532	CB	BCYS	B	381	1.830	6.406	15.226	0.25	16.63
ATOM	2533	SG	ACYS	B	381	1.167	7.518	14.060	0.75	33.54
ATOM	2534	SG	BCYS	B	381	3.048	5.656	14.128	0.25	10.36
ATOM	2535	C	ACYS	B	381	1.626	4.269	16.592	0.75	20.59
ATOM	2536	C	BCYS	B	381	1.689	4.305	16.561	0.25	19.19
ATOM	2537	O	ACYS	B	381	1.737	3.161	16.069	0.75	19.16
ATOM	2538	O	BCYS	B	381	1.904	3.241	15.982	0.25	19.25
ATOM	2539	N	ALA	B	382	2.134	4.560	17.785	1.00	19.04
ATOM	2540	CA	ALA	B	382	2.955	3.602	18.530	1.00	20.27
ATOM	2541	CB	ALA	B	382	4.135	4.364	19.143	1.00	18.68
ATOM	2542	C	ALA	B	382	2.356	2.702	19.607	1.00	16.82
ATOM	2543	O	ALA	B	382	3.070	1.852	20.142	1.00	13.37
ATOM	2544	N	TRP	B	383	1.074	2.855	19.916	1.00	15.30
ATOM	2545	CA	TRP	B	383	0.487	2.089	21.013	1.00	15.80
ATOM	2546	CB	TRP	B	383	-1.009	2.410	21.160	1.00	16.63
ATOM	2547	CG	TRP	B	383	-1.871	1.775	20.129	1.00	19.93
ATOM	2548	CD2	TRP	B	383	-2.493	0.483	20.198	1.00	20.80
ATOM	2549	CE2	TRP	B	383	-3.226	0.309	19.003	1.00	19.27
ATOM	2550	CE3	TRP	B	383	-2.506	-0.542	21.155	1.00	21.32
ATOM	2551	CD1	TRP	B	383	-2.236	2.312	18.933	1.00	18.59
ATOM	2552	NE1	TRP	B	383	-3.051	1.439	18.250	1.00	23.67
ATOM	2553	CZ2	TRP	B	383	-3.963	-0.853	18.733	1.00	21.55
ATOM	2554	CZ3	TRP	B	383	-3.243	-1.702	20.888	1.00	20.29
ATOM	2555	CH2	TRP	B	383	-3.960	-1.844	19.686	1.00	19.03
ATOM	2556	C	TRP	B	383	0.701	0.579	21.020	1.00	17.35
ATOM	2557	O	TRP	B	383	0.982	0.010	22.077	1.00	13.92
ATOM	2558	N	LEU	B	384	0.568	-0.087	19.879	1.00	14.07
ATOM	2559	CA	LEU	B	384	0.773	-1.532	19.903	1.00	15.98
ATOM	2560	CB	LEU	B	384	0.181	-2.200	18.656	1.00	12.19
ATOM	2561	CG	LEU	B	384	0.173	-3.735	18.720	1.00	12.97
ATOM	2562	CD1	LEU	B	384	-0.352	-4.240	20.089	1.00	10.65
ATOM	2563	CD2	LEU	B	384	-0.707	-4.259	17.586	1.00	17.84
ATOM	2564	C	LEU	B	384	2.262	-1.861	20.034	1.00	14.64
ATOM	2565	O	LEU	B	384	2.627	-2.833	20.690	1.00	13.78
ATOM	2566	N	GLU	B	385	3.116	-1.046	19.414	1.00	14.96
ATOM	2567	CA	GLU	B	385	4.565	-1.260	19.509	1.00	13.79
ATOM	2568	CB	GLU	B	385	5.336	-0.179	18.739	1.00	15.34
ATOM	2569	CG	GLU	B	385	5.297	-0.312	17.207	1.00	15.38
ATOM	2570	CD	GLU	B	385	6.162	0.738	16.520	1.00	23.97
ATOM	2571	OE1	GLU	B	385	7.381	0.500	16.358	1.00	21.03
ATOM	2572	OE2	GLU	B	385	5.622	1.808	16.149	1.00	22.19
ATOM	2573	C	GLU	B	385	4.963	-1.161	20.987	1.00	15.79
ATOM	2574	O	GLU	B	385	5.788	-1.942	21.463	1.00	15.04
ATOM	2575	N	ILE	B	386	4.389	-0.213	21.690	1.00	13.32
ATOM	2576	CA	ILE	B	386	4.723	-0.019	23.108	1.00	14.06
ATOM	2577	CB	ILE	B	386	4.173	1.326	23.614	1.00	15.36
ATOM	2578	CG2	ILE	B	386	4.374	1.451	25.130	1.00	15.97
ATOM	2579	CG1	ILE	B	386	4.910	2.476	22.907	1.00	17.95

	ATOM	2580	CD1	ILE	B	386	4.118	3.768	22.874	1.00	21.12
	ATOM	2581	C	ILE	B	386	4.227	-1.164	23.993	1.00	14.97
	ATOM	2582	O	ILE	B	386	4.905	-1.560	24.941	1.00	19.60
	ATOM	2583	N	LEU	B	387	3.038	-1.675	23.709	1.00	15.18
5	ATOM	2584	CA	LEU	B	387	2.516	-2.791	24.478	1.00	15.98
	ATOM	2585	CB	LEU	B	387	1.070	-3.097	24.080	1.00	17.15
	ATOM	2586	CG	LEU	B	387	-0.031	-2.113	24.486	1.00	19.65
	ATOM	2587	CD1	LEU	B	387	-1.371	-2.628	23.972	1.00	17.77
	ATOM	2588	CD2	LEU	B	387	-0.075	-1.966	26.002	1.00	15.38
10	ATOM	2589	C	LEU	B	387	3.391	-4.013	24.180	1.00	14.69
	ATOM	2590	O	LEU	B	387	3.712	-4.792	25.076	1.00	14.03
	ATOM	2591	N	MET	B	388	3.785	-4.178	22.921	1.00	16.43
	ATOM	2592	CA	MET	B	388	4.602	-5.329	22.547	1.00	16.67
	ATOM	2593	CB	MET	B	388	4.673	-5.460	21.026	1.00	14.83
15	ATOM	2594	CG	MET	B	388	3.403	-6.066	20.453	1.00	13.91
	ATOM	2595	SD	MET	B	388	3.364	-6.193	18.675	1.00	17.23
	ATOM	2596	CE	MET	B	388	1.906	-7.225	18.511	1.00	14.97
	ATOM	2597	C	MET	B	388	6.004	-5.332	23.133	1.00	20.19
	ATOM	2598	O	MET	B	388	6.460	-6.366	23.636	1.00	21.50
20	ATOM	2599	N	ILE	B	389	6.707	-4.203	23.074	1.00	15.34
	ATOM	2600	CA	ILE	B	389	8.044	-4.209	23.634	1.00	15.59
	ATOM	2601	CB	ILE	B	389	8.836	-2.911	23.322	1.00	14.95
	ATOM	2602	CG2	ILE	B	389	8.330	-1.746	24.158	1.00	12.81
	ATOM	2603	CG1	ILE	B	389	10.325	-3.164	23.602	1.00	17.24
25	ATOM	2604	CD1	ILE	B	389	11.228	-1.972	23.357	1.00	15.65
	ATOM	2605	C	ILE	B	389	7.950	-4.446	25.147	1.00	14.30
	ATOM	2606	O	ILE	B	389	8.844	-5.044	25.739	1.00	18.72
	ATOM	2607	N	GLY	B	390	6.855	-4.007	25.761	1.00	13.99
	ATOM	2608	CA	GLY	B	390	6.681	-4.219	27.189	1.00	14.87
30	ATOM	2609	C	GLY	B	390	6.444	-5.702	27.463	1.00	18.54
	ATOM	2610	O	GLY	B	390	6.989	-6.282	28.403	1.00	16.54
	ATOM	2611	N	LEU	B	391	5.623	-6.325	26.628	1.00	16.15
	ATOM	2612	CA	LEU	B	391	5.334	-7.743	26.775	1.00	18.91
	ATOM	2613	CB	LEU	B	391	4.332	-8.179	25.699	1.00	19.55
35	ATOM	2614	CG	LEU	B	391	4.157	-9.689	25.457	1.00	20.91
	ATOM	2615	CD1	LEU	B	391	3.580	-10.351	26.699	1.00	19.41
	ATOM	2616	CD2	LEU	B	391	3.232	-9.913	24.268	1.00	20.70
	ATOM	2617	C	LEU	B	391	6.649	-8.518	26.625	1.00	20.31
	ATOM	2618	O	LEU	B	391	7.002	-9.352	27.465	1.00	18.66
40	ATOM	2619	N	VAL	B	392	7.378	-8.215	25.557	1.00	18.71
	ATOM	2620	CA	VAL	B	392	8.649	-8.868	25.278	1.00	19.51
	ATOM	2621	CB	VAL	B	392	9.288	-8.281	24.005	1.00	23.77
	ATOM	2622	CG1	VAL	B	392	10.751	-8.687	23.920	1.00	24.63
	ATOM	2623	CG2	VAL	B	392	8.520	-8.773	22.767	1.00	19.94
45	ATOM	2624	C	VAL	B	392	9.615	-8.707	26.450	1.00	22.80
	ATOM	2625	O	VAL	B	392	10.336	-9.637	26.811	1.00	19.36
	ATOM	2626	N	TRP	B	393	9.617	-7.522	27.046	1.00	22.10
	ATOM	2627	CA	TRP	B	393	10.492	-7.241	28.171	1.00	23.20

	ATOM	2628	CB	TRP	B	393	10.388	-5.773	28.578	1.00	19.22
	ATOM	2629	CG	TRP	B	393	11.056	-5.479	29.895	1.00	22.53
	ATOM	2630	CD2	TRP	B	393	12.453	-5.591	30.193	1.00	20.36
	ATOM	2631	CE2	TRP	B	393	12.624	-5.208	31.545	1.00	25.65
	ATOM	2632	CE3	TRP	B	393	13.578	-5.976	29.449	1.00	22.12
	ATOM	2633	CD1	TRP	B	393	10.452	-5.046	31.044	1.00	23.02
	ATOM	2634	NE1	TRP	B	393	11.387	-4.881	32.037	1.00	24.91
	ATOM	2635	CZ2	TRP	B	393	13.876	-5.200	32.171	1.00	23.00
	ATOM	2636	CZ3	TRP	B	393	14.829	-5.968	30.072	1.00	23.98
	ATOM	2637	CH2	TRP	B	393	14.964	-5.582	31.423	1.00	23.20
	ATOM	2638	C	TRP	B	393	10.208	-8.114	29.388	1.00	24.36
	ATOM	2639	O	TRP	B	393	11.128	-8.717	29.944	1.00	23.04
	ATOM	2640	N	ARG	B	394	8.952	-8.189	29.819	1.00	21.29
	ATOM	2641	CA	ARG	B	394	8.680	-9.003	30.990	1.00	22.43
	ATOM	2642	CB	ARG	B	394	7.365	-8.601	31.667	1.00	23.97
	ATOM	2643	CG	ARG	B	394	6.259	-8.149	30.759	1.00	26.16
	ATOM	2644	CD	ARG	B	394	5.026	-7.727	31.574	1.00	20.86
	ATOM	2645	NE	ARG	B	394	3.817	-7.937	30.786	1.00	19.54
	ATOM	2646	CZ	ARG	B	394	3.327	-7.059	29.915	1.00	20.58
	ATOM	2647	NH1	ARG	B	394	3.944	-5.902	29.722	1.00	17.41
	ATOM	2648	NH2	ARG	B	394	2.229	-7.347	29.220	1.00	16.82
	ATOM	2649	C	ARG	B	394	8.695	-10.502	30.713	1.00	21.78
	ATOM	2650	O	ARG	B	394	8.657	-11.294	31.648	1.00	23.44
	ATOM	2651	N	SER	B	395	8.767	-10.880	29.438	1.00	17.10
	ATOM	2652	CA	SER	B	395	8.805	-12.289	29.041	1.00	25.08
	ATOM	2653	CB	SER	B	395	8.206	-12.473	27.638	1.00	19.47
	ATOM	2654	OG	SER	B	395	6.832	-12.136	27.619	1.00	21.73
	ATOM	2655	C	SER	B	395	10.239	-12.831	29.031	1.00	26.29
	ATOM	2656	O	SER	B	395	10.458	-14.030	28.854	1.00	23.75
	ATOM	2657	N	MET	B	396	11.206	-11.938	29.210	1.00	30.79
	ATOM	2658	CA	MET	B	396	12.620	-12.307	29.205	1.00	35.07
	ATOM	2659	CB	MET	B	396	13.479	-11.063	29.423	1.00	33.84
	ATOM	2660	CG	MET	B	396	14.155	-10.569	28.171	1.00	36.88
	ATOM	2661	SD	MET	B	396	15.149	-9.127	28.491	1.00	40.96
	ATOM	2662	CE	MET	B	396	16.675	-9.849	28.998	1.00	39.67
	ATOM	2663	C	MET	B	396	12.983	-13.353	30.250	1.00	35.88
	ATOM	2664	O	MET	B	396	13.828	-14.215	30.011	1.00	34.52
	ATOM	2665	N	GLU	B	397	12.348	-13.266	31.410	1.00	36.19
	ATOM	2666	CA	GLU	B	397	12.604	-14.206	32.492	1.00	39.24
	ATOM	2667	CB	GLU	B	397	12.153	-13.605	33.821	1.00	44.38
	ATOM	2668	CG	GLU	B	397	12.983	-12.422	34.271	1.00	54.05
	ATOM	2669	CD	GLU	B	397	13.483	-12.587	35.686	1.00	56.78
	ATOM	2670	OE1	GLU	B	397	13.380	-11.621	36.470	1.00	60.90
	ATOM	2671	OE2	GLU	B	397	13.975	-13.688	36.013	1.00	60.82
	ATOM	2672	C	GLU	B	397	11.878	-15.528	32.273	1.00	36.65
	ATOM	2673	O	GLU	B	397	12.021	-16.459	33.061	1.00	35.84
	ATOM	2674	N	HIS	B	398	11.100	-15.609	31.202	1.00	32.14
	ATOM	2675	CA	HIS	B	398	10.347	-16.823	30.914	1.00	29.48

	ATOM	2676	CB	HIS	B	398	8.863	-16.567	31.178	1.00	29.87
	ATOM	2677	CG	HIS	B	398	8.582	-16.111	32.574	1.00	31.80
	ATOM	2678	CD2	HIS	B	398	8.215	-16.801	33.678	1.00	29.12
	ATOM	2679	ND1	HIS	B	398	8.727	-14.799	32.972	1.00	33.27
5	ATOM	2680	CE1	HIS	B	398	8.462	-14.701	34.262	1.00	32.19
	ATOM	2681	NE2	HIS	B	398	8.148	-15.902	34.714	1.00	33.48
	ATOM	2682	C	HIS	B	398	10.556	-17.317	29.492	1.00	25.95
	ATOM	2683	O	HIS	B	398	9.637	-17.291	28.672	1.00	27.47
	ATOM	2684	N	PRO	B	399	11.771	-17.801	29.186	1.00	29.09
10	ATOM	2685	CD	PRO	B	399	12.926	-17.922	30.096	1.00	29.93
	ATOM	2686	CA	PRO	B	399	12.079	-18.300	27.845	1.00	27.40
	ATOM	2687	CB	PRO	B	399	13.434	-18.988	28.016	1.00	32.09
	ATOM	2688	CG	PRO	B	399	14.062	-18.284	29.170	1.00	30.81
	ATOM	2689	C	PRO	B	399	11.009	-19.246	27.319	1.00	29.76
15	ATOM	2690	O	PRO	B	399	10.552	-20.137	28.035	1.00	29.18
	ATOM	2691	N	GLY	B	400	10.601	-19.035	26.071	1.00	27.45
	ATOM	2692	CA	GLY	B	400	9.588	-19.884	25.466	1.00	26.93
	ATOM	2693	C	GLY	B	400	8.161	-19.537	25.849	1.00	26.73
	ATOM	2694	O	GLY	B	400	7.220	-20.153	25.356	1.00	28.36
20	ATOM	2695	N	LYS	B	401	7.996	-18.554	26.727	1.00	25.50
	ATOM	2696	CA	LYS	B	401	6.668	-18.139	27.165	1.00	23.45
	ATOM	2697	CB	LYS	B	401	6.435	-18.563	28.619	1.00	28.50
	ATOM	2698	CG	LYS	B	401	6.476	-20.069	28.879	1.00	28.58
	ATOM	2699	CD	LYS	B	401	6.181	-20.353	30.349	1.00	35.47
25	ATOM	2700	CE	LYS	B	401	6.073	-21.847	30.635	1.00	38.59
	ATOM	2701	NZ	LYS	B	401	7.177	-22.611	29.989	1.00	42.39
	ATOM	2702	C	LYS	B	401	6.493	-16.622	27.060	1.00	21.78
	ATOM	2703	O	LYS	B	401	7.465	-15.872	27.035	1.00	21.45
	ATOM	2704	N	LEU	B	402	5.241	-16.181	26.995	1.00	23.45
30	ATOM	2705	CA	LEU	B	402	4.929	-14.759	26.925	1.00	21.37
	ATOM	2706	CB	LEU	B	402	4.088	-14.449	25.689	1.00	18.47
	ATOM	2707	CG	LEU	B	402	4.798	-14.673	24.360	1.00	16.89
	ATOM	2708	CD1	LEU	B	402	3.821	-14.395	23.211	1.00	21.23
	ATOM	2709	CD2	LEU	B	402	6.011	-13.760	24.277	1.00	23.15
35	ATOM	2710	C	LEU	B	402	4.147	-14.399	28.179	1.00	19.66
	ATOM	2711	O	LEU	B	402	3.024	-14.880	28.381	1.00	18.05
	ATOM	2712	N	LEU	B	403	4.743	-13.559	29.019	1.00	19.54
	ATOM	2713	CA	LEU	B	403	4.099	-13.148	30.259	1.00	20.21
	ATOM	2714	CB	LEU	B	403	5.155	-12.856	31.332	1.00	23.16
40	ATOM	2715	CG	LEU	B	403	4.639	-12.682	32.766	1.00	29.54
	ATOM	2716	CD1	LEU	B	403	5.519	-13.450	33.728	1.00	32.67
	ATOM	2717	CD2	LEU	B	403	4.626	-11.213	33.138	1.00	32.38
	ATOM	2718	C	LEU	B	403	3.219	-11.918	30.043	1.00	20.42
	ATOM	2719	O	LEU	B	403	3.638	-10.787	30.291	1.00	19.18
45	ATOM	2720	N	PHE	B	404	2.003	-12.145	29.565	1.00	21.44
	ATOM	2721	CA	PHE	B	404	1.066	-11.053	29.340	1.00	21.69
	ATOM	2722	CB	PHE	B	404	-0.199	-11.598	28.687	1.00	17.26
	ATOM	2723	CG	PHE	B	404	-0.026	-11.897	27.227	1.00	19.75

ATOM	2724	CD1	PHE	B	404	0.364	-13.167	26.801	1.00	17.90
ATOM	2725	CD2	PHE	B	404	-0.210	-10.897	26.280	1.00	17.04
ATOM	2726	CE1	PHE	B	404	0.572	-13.434	25.447	1.00	19.88
ATOM	2727	CE2	PHE	B	404	-0.007	-11.148	24.924	1.00	18.47
ATOM	2728	CZ	PHE	B	404	0.386	-12.418	24.503	1.00	16.45
ATOM	2729	C	PHE	B	404	0.768	-10.403	30.685	1.00	21.95
ATOM	2730	O	PHE	B	404	0.656	-9.177	30.804	1.00	22.99
ATOM	2731	N	ALA	B	405	0.670	-11.247	31.702	1.00	21.12
ATOM	2732	CA	ALA	B	405	0.424	-10.814	33.066	1.00	22.43
ATOM	2733	CB	ALA	B	405	-1.074	-10.603	33.304	1.00	24.69
ATOM	2734	C	ALA	B	405	0.959	-11.926	33.962	1.00	22.40
ATOM	2735	O	ALA	B	405	1.133	-13.061	33.517	1.00	21.67
ATOM	2736	N	PRO	B	406	1.246	-11.612	35.230	1.00	25.60
ATOM	2737	CD	PRO	B	406	1.129	-10.294	35.878	1.00	23.65
ATOM	2738	CA	PRO	B	406	1.765	-12.632	36.148	1.00	25.91
ATOM	2739	CB	PRO	B	406	1.899	-11.882	37.475	1.00	27.04
ATOM	2740	CG	PRO	B	406	2.017	-10.431	37.068	1.00	26.56
ATOM	2741	C	PRO	B	406	0.876	-13.873	36.259	1.00	25.12
ATOM	2742	O	PRO	B	406	1.368	-14.967	36.538	1.00	28.92
ATOM	2743	N	ASN	B	407	-0.426	-13.713	36.039	1.00	23.53
ATOM	2744	CA	ASN	B	407	-1.345	-14.852	36.109	1.00	24.09
ATOM	2745	CB	ASN	B	407	-2.553	-14.526	36.986	1.00	24.08
ATOM	2746	CG	ASN	B	407	-3.327	-13.328	36.486	1.00	26.72
ATOM	2747	OD1	ASN	B	407	-2.851	-12.574	35.635	1.00	22.65
ATOM	2748	ND2	ASN	B	407	-4.528	-13.140	37.019	1.00	26.46
ATOM	2749	C	ASN	B	407	-1.820	-15.231	34.714	1.00	26.91
ATOM	2750	O	ASN	B	407	-2.859	-15.870	34.548	1.00	28.68
ATOM	2751	N	LEU	B	408	-1.059	-14.816	33.708	1.00	27.28
ATOM	2752	CA	LEU	B	408	-1.387	-15.124	32.327	1.00	27.23
ATOM	2753	CB	LEU	B	408	-2.247	-14.030	31.699	1.00	26.61
ATOM	2754	CG	LEU	B	408	-2.815	-14.464	30.341	1.00	27.51
ATOM	2755	CD1	LEU	B	408	-3.702	-15.692	30.546	1.00	28.75
ATOM	2756	CD2	LEU	B	408	-3.598	-13.330	29.694	1.00	25.48
ATOM	2757	C	LEU	B	408	-0.113	-15.316	31.514	1.00	27.56
ATOM	2758	O	LEU	B	408	0.247	-14.465	30.695	1.00	26.86
ATOM	2759	N	LEU	B	409	0.553	-16.426	31.759	1.00	27.54
ATOM	2760	CA	LEU	B	409	1.786	-16.774	31.065	1.00	31.96
ATOM	2761	CB	LEU	B	409	2.786	-17.355	32.058	1.00	31.88
ATOM	2762	CG	LEU	B	409	4.186	-17.703	31.562	1.00	37.72
ATOM	2763	CD1	LEU	B	409	4.773	-16.551	30.770	1.00	39.57
ATOM	2764	CD2	LEU	B	409	5.066	-18.018	32.758	1.00	41.72
ATOM	2765	C	LEU	B	409	1.401	-17.805	30.009	1.00	31.53
ATOM	2766	O	LEU	B	409	0.921	-18.892	30.340	1.00	32.67
ATOM	2767	N	LEU	B	410	1.604	-17.465	28.746	1.00	29.58
ATOM	2768	CA	LEU	B	410	1.228	-18.361	27.660	1.00	31.55
ATOM	2769	CB	LEU	B	410	0.192	-17.672	26.762	1.00	29.83
ATOM	2770	CG	LEU	B	410	-1.047	-17.080	27.452	1.00	28.55
ATOM	2771	CD1	LEU	B	410	-1.770	-16.135	26.501	1.00	26.92

	ATOM	2772	CD2	LEU	B	410	-1.979	-18.200	27.891	1.00	30.49
	ATOM	2773	C	LEU	B	410	2.397	-18.839	26.814	1.00	33.88
	ATOM	2774	O	LEU	B	410	3.427	-18.170	26.726	1.00	36.49
	ATOM	2775	N	ASP	B	411	2.238	-20.013	26.206	1.00	38.80
5	ATOM	2776	CA	ASP	B	411	3.275	-20.562	25.336	1.00	38.39
	ATOM	2777	CB	ASP	B	411	3.657	-21.990	25.752	1.00	44.53
	ATOM	2778	CG	ASP	B	411	2.476	-22.943	25.749	1.00	44.90
	ATOM	2779	OD1	ASP	B	411	1.773	-23.035	24.719	1.00	45.70
	ATOM	2780	OD2	ASP	B	411	2.254	-23.603	26.786	1.00	50.54
10	ATOM	2781	C	ASP	B	411	2.745	-20.551	23.909	1.00	38.57
	ATOM	2782	O	ASP	B	411	1.549	-20.341	23.686	1.00	36.48
	ATOM	2783	N	ARG	B	412	3.635	-20.777	22.949	1.00	36.85
	ATOM	2784	CA	ARG	B	412	3.259	-20.763	21.541	1.00	38.32
	ATOM	2785	CB	ARG	B	412	4.488	-21.083	20.675	1.00	38.69
15	ATOM	2786	CG	ARG	B	412	4.361	-22.314	19.799	1.00	40.05
	ATOM	2787	CD	ARG	B	412	5.644	-22.552	19.012	1.00	42.98
	ATOM	2788	NE	ARG	B	412	5.540	-22.099	17.626	1.00	40.95
	ATOM	2789	CZ	ARG	B	412	4.649	-22.559	16.753	1.00	41.11
	ATOM	2790	NH1	ARG	B	412	3.777	-23.490	17.115	1.00	44.01
20	ATOM	2791	NH2	ARG	B	412	4.632	-22.091	15.515	1.00	41.28
	ATOM	2792	C	ARG	B	412	2.107	-21.712	21.217	1.00	37.64
	ATOM	2793	O	ARG	B	412	1.287	-21.427	20.343	1.00	36.51
	ATOM	2794	N	ASN	B	413	2.041	-22.834	21.923	1.00	35.32
	ATOM	2795	CA	ASN	B	413	0.974	-23.798	21.688	1.00	36.68
25	ATOM	2796	CB	ASN	B	413	1.170	-25.035	22.570	1.00	37.54
	ATOM	2797	CG	ASN	B	413	2.017	-26.100	21.901	1.00	43.56
	ATOM	2798	OD1	ASN	B	413	2.309	-26.022	20.704	1.00	46.11
	ATOM	2799	ND2	ASN	B	413	2.418	-27.104	22.671	1.00	47.04
	ATOM	2800	C	ASN	B	413	-0.383	-23.168	21.982	1.00	34.01
30	ATOM	2801	O	ASN	B	413	-1.349	-23.372	21.247	1.00	32.43
	ATOM	2802	N	GLN	B	414	-0.447	-22.397	23.063	1.00	32.85
	ATOM	2803	CA	GLN	B	414	-1.685	-21.741	23.449	1.00	31.91
	ATOM	2804	CB	GLN	B	414	-1.558	-21.172	24.863	1.00	33.17
	ATOM	2805	CG	GLN	B	414	-1.528	-22.242	25.948	1.00	32.31
35	ATOM	2806	CD	GLN	B	414	-1.293	-21.667	27.327	1.00	34.63
	ATOM	2807	OE1	GLN	B	414	-0.176	-21.277	27.666	1.00	33.23
	ATOM	2808	NE2	GLN	B	414	-2.349	-21.606	28.131	1.00	34.56
	ATOM	2809	C	GLN	B	414	-2.052	-20.638	22.463	1.00	29.57
	ATOM	2810	O	GLN	B	414	-3.195	-20.204	22.409	1.00	31.32
40	ATOM	2811	N	GLY	B	415	-1.077	-20.190	21.682	1.00	30.96
	ATOM	2812	CA	GLY	B	415	-1.350	-19.160	20.697	1.00	34.27
	ATOM	2813	C	GLY	B	415	-2.184	-19.725	19.562	1.00	35.27
	ATOM	2814	O	GLY	B	415	-2.918	-19.000	18.887	1.00	33.20
	ATOM	2815	N	LYS	B	416	-2.070	-21.031	19.354	1.00	35.28
45	ATOM	2816	CA	LYS	B	416	-2.819	-21.707	18.299	1.00	38.26
	ATOM	2817	CB	LYS	B	416	-2.398	-23.177	18.201	1.00	38.00
	ATOM	2818	CG	LYS	B	416	-0.973	-23.407	17.736	1.00	40.05
	ATOM	2819	CD	LYS	B	416	-0.405	-24.668	18.369	1.00	44.10

ATOM	2820	CE	LYS	B	416	0.306	-25.541	17.346	1.00	41.85
ATOM	2821	NZ	LYS	B	416	1.286	-24.760	16.542	1.00	45.63
ATOM	2822	C	LYS	B	416	-4.321	-21.645	18.559	1.00	36.93
ATOM	2823	O	LYS	B	416	-5.121	-21.790	17.638	1.00	38.36
ATOM	2824	N	CYS	B	417	-4.698	-21.430	19.817	1.00	37.10
ATOM	2825	CA	CYS	B	417	-6.106	-21.371	20.196	1.00	36.46
ATOM	2826	CB	CYS	B	417	-6.218	-21.226	21.717	1.00	39.01
ATOM	2827	SG	CYS	B	417	-5.674	-22.710	22.612	1.00	43.81
ATOM	2828	C	CYS	B	417	-6.899	-20.277	19.491	1.00	35.19
ATOM	2829	O	CYS	B	417	-8.127	-20.296	19.485	1.00	33.92
ATOM	2830	N	VAL	B	418	-6.195	-19.316	18.906	1.00	36.04
ATOM	2831	CA	VAL	B	418	-6.838	-18.236	18.163	1.00	34.59
ATOM	2832	CB	VAL	B	418	-6.525	-16.850	18.775	1.00	34.87
ATOM	2833	CG1	VAL	B	418	-6.831	-15.763	17.765	1.00	35.32
ATOM	2834	CG2	VAL	B	418	-7.350	-16.630	20.036	1.00	33.65
ATOM	2835	C	VAL	B	418	-6.241	-18.317	16.764	1.00	34.17
ATOM	2836	O	VAL	B	418	-5.020	-18.323	16.611	1.00	32.73
ATOM	2837	N	GLU	B	419	-7.084	-18.388	15.740	1.00	33.44
ATOM	2838	CA	GLU	B	419	-6.554	-18.500	14.390	1.00	34.52
ATOM	2839	CB	GLU	B	419	-7.681	-18.722	13.380	1.00	36.21
ATOM	2840	CG	GLU	B	419	-8.597	-17.538	13.166	1.00	44.19
ATOM	2841	CD	GLU	B	419	-9.477	-17.723	11.946	1.00	48.47
ATOM	2842	OE1	GLU	B	419	-9.157	-18.605	11.119	1.00	51.04
ATOM	2843	OE2	GLU	B	419	-10.484	-16.993	11.813	1.00	48.91
ATOM	2844	C	GLU	B	419	-5.717	-17.289	13.997	1.00	32.89
ATOM	2845	O	GLU	B	419	-6.156	-16.144	14.123	1.00	31.09
ATOM	2846	N	GLY	B	420	-4.501	-17.562	13.535	1.00	32.84
ATOM	2847	CA	GLY	B	420	-3.594	-16.506	13.122	1.00	34.37
ATOM	2848	C	GLY	B	420	-2.722	-15.955	14.240	1.00	35.30
ATOM	2849	O	GLY	B	420	-1.745	-15.246	13.975	1.00	35.94
ATOM	2850	N	MET	B	421	-3.052	-16.285	15.486	1.00	30.08
ATOM	2851	CA	MET	B	421	-2.289	-15.780	16.625	1.00	29.22
ATOM	2852	CB	MET	B	421	-3.108	-15.922	17.914	1.00	22.54
ATOM	2853	CG	MET	B	421	-2.469	-15.270	19.124	1.00	23.82
ATOM	2854	SD	MET	B	421	-2.124	-13.494	18.872	1.00	28.40
ATOM	2855	CE	MET	B	421	-3.697	-12.800	19.233	1.00	24.67
ATOM	2856	C	MET	B	421	-0.912	-16.416	16.821	1.00	29.67
ATOM	2857	O	MET	B	421	0.022	-15.751	17.269	1.00	29.76
ATOM	2858	N	VAL	B	422	-0.766	-17.694	16.484	1.00	30.63
ATOM	2859	CA	VAL	B	422	0.524	-18.338	16.675	1.00	29.90
ATOM	2860	CB	VAL	B	422	0.482	-19.835	16.273	1.00	35.74
ATOM	2861	CG1	VAL	B	422	0.514	-19.992	14.753	1.00	37.64
ATOM	2862	CG2	VAL	B	422	1.659	-20.555	16.897	1.00	31.68
ATOM	2863	C	VAL	B	422	1.669	-17.640	15.935	1.00	28.64
ATOM	2864	O	VAL	B	422	2.788	-17.571	16.441	1.00	26.15
ATOM	2865	N	GLU	B	423	1.402	-17.113	14.747	1.00	28.70
ATOM	2866	CA	GLU	B	423	2.454	-16.435	13.997	1.00	31.34
ATOM	2867	CB	GLU	B	423	1.963	-16.050	12.596	1.00	36.21

	ATOM	2868	CG	GLU	B	423	0.502	-16.376	12.325	1.00	45.83
	ATOM	2869	CD	GLU	B	423	0.250	-17.865	12.144	1.00	46.71
	ATOM	2870	OE1	GLU	B	423	-0.746	-18.368	12.706	1.00	45.97
	ATOM	2871	OE2	GLU	B	423	1.045	-18.530	11.442	1.00	50.05
5	ATOM	2872	C	GLU	B	423	2.928	-15.186	14.744	1.00	30.57
	ATOM	2873	O	GLU	B	423	4.119	-14.870	14.759	1.00	26.59
	ATOM	2874	N	ILE	B	424	2.001	-14.478	15.378	1.00	26.19
	ATOM	2875	CA	ILE	B	424	2.381	-13.279	16.111	1.00	26.23
	ATOM	2876	CB	ILE	B	424	1.134	-12.435	16.452	1.00	29.33
10	ATOM	2877	CG2	ILE	B	424	1.492	-11.315	17.425	1.00	30.91
	ATOM	2878	CG1	ILE	B	424	0.584	-11.817	15.160	1.00	29.09
	ATOM	2879	CD1	ILE	B	424	-0.895	-11.514	15.187	1.00	30.51
	ATOM	2880	C	ILE	B	424	3.153	-13.673	17.370	1.00	24.22
	ATOM	2881	O	ILE	B	424	4.152	-13.037	17.725	1.00	21.05
15	ATOM	2882	N	PHE	B	425	2.708	-14.746	18.023	1.00	21.71
	ATOM	2883	CA	PHE	B	425	3.370	-15.236	19.223	1.00	18.85
	ATOM	2884	CB	PHE	B	425	2.650	-16.479	19.768	1.00	22.98
	ATOM	2885	CG	PHE	B	425	1.580	-16.183	20.795	1.00	22.17
	ATOM	2886	CD1	PHE	B	425	1.287	-17.112	21.792	1.00	25.47
20	ATOM	2887	CD2	PHE	B	425	0.843	-15.001	20.747	1.00	26.30
	ATOM	2888	CE1	PHE	B	425	0.273	-16.871	22.724	1.00	24.33
	ATOM	2889	CE2	PHE	B	425	-0.174	-14.749	21.676	1.00	25.03
	ATOM	2890	CZ	PHE	B	425	-0.459	-15.684	22.663	1.00	26.44
	ATOM	2891	C	PHE	B	425	4.817	-15.610	18.885	1.00	20.00
25	ATOM	2892	O	PHE	B	425	5.741	-15.292	19.636	1.00	21.15
	ATOM	2893	N	ASP	B	426	5.023	-16.281	17.754	1.00	19.87
	ATOM	2894	CA	ASP	B	426	6.378	-16.685	17.377	1.00	23.20
	ATOM	2895	CB	ASP	B	426	6.364	-17.510	16.090	1.00	26.53
	ATOM	2896	CG	ASP	B	426	5.992	-18.965	16.335	1.00	34.28
30	ATOM	2897	OD1	ASP	B	426	6.242	-19.467	17.455	1.00	35.24
	ATOM	2898	OD2	ASP	B	426	5.448	-19.600	15.409	1.00	31.49
	ATOM	2899	C	ASP	B	426	7.302	-15.489	17.198	1.00	21.84
	ATOM	2900	O	ASP	B	426	8.465	-15.526	17.593	1.00	21.55
	ATOM	2901	N	MET	B	427	6.788	-14.429	16.591	1.00	20.12
35	ATOM	2902	CA	MET	B	427	7.597	-13.234	16.382	1.00	21.02
	ATOM	2903	CB	MET	B	427	6.836	-12.228	15.520	1.00	18.53
	ATOM	2904	CG	MET	B	427	6.864	-12.559	14.038	1.00	27.92
	ATOM	2905	SD	MET	B	427	6.011	-11.341	13.024	1.00	32.84
	ATOM	2906	CE	MET	B	427	4.363	-11.532	13.581	1.00	33.63
40	ATOM	2907	C	MET	B	427	7.945	-12.616	17.732	1.00	17.42
	ATOM	2908	O	MET	B	427	9.073	-12.180	17.950	1.00	22.09
	ATOM	2909	N	LEU	B	428	6.968	-12.597	18.634	1.00	20.47
	ATOM	2910	CA	LEU	B	428	7.157	-12.033	19.968	1.00	20.13
	ATOM	2911	CB	LEU	B	428	5.812	-11.964	20.706	1.00	17.58
45	ATOM	2912	CG	LEU	B	428	4.852	-10.887	20.179	1.00	18.41
	ATOM	2913	CD1	LEU	B	428	3.443	-11.155	20.687	1.00	11.95
	ATOM	2914	CD2	LEU	B	428	5.324	-9.505	20.631	1.00	17.80
	ATOM	2915	C	LEU	B	428	8.159	-12.856	20.767	1.00	20.68

	ATOM	2916	O	LEU	B	428	9.028	-12.305	21.445	1.00	20.45
	ATOM	2917	N	LEU	B	429	8.037	-14.178	20.679	1.00	20.35
	ATOM	2918	CA	LEU	B	429	8.938	-15.082	21.382	1.00	19.82
	ATOM	2919	CB	LEU	B	429	8.470	-16.532	21.211	1.00	23.13
5	ATOM	2920	CG	LEU	B	429	7.189	-16.839	21.997	1.00	21.85
	ATOM	2921	CD1	LEU	B	429	6.551	-18.123	21.494	1.00	25.39
	ATOM	2922	CD2	LEU	B	429	7.537	-16.944	23.475	1.00	24.91
	ATOM	2923	C	LEU	B	429	10.361	-14.936	20.865	1.00	20.74
	ATOM	2924	O	LEU	B	429	11.318	-14.968	21.638	1.00	21.02
10	ATOM	2925	N	ALA	B	430	10.495	-14.770	19.554	1.00	21.40
	ATOM	2926	CA	ALA	B	430	11.808	-14.609	18.947	1.00	22.77
	ATOM	2927	CB	ALA	B	430	11.677	-14.596	17.432	1.00	21.11
	ATOM	2928	C	ALA	B	430	12.467	-13.315	19.440	1.00	22.40
	ATOM	2929	O	ALA	B	430	13.670	-13.277	19.713	1.00	20.62
15	ATOM	2930	N	THR	B	431	11.670	-12.258	19.567	1.00	21.09
	ATOM	2931	CA	THR	B	431	12.183	-10.974	20.021	1.00	22.67
	ATOM	2932	CB	THR	B	431	11.128	-9.866	19.863	1.00	23.77
	ATOM	2933	OG1	THR	B	431	10.572	-9.936	18.547	1.00	23.84
	ATOM	2934	CG2	THR	B	431	11.762	-8.489	20.073	1.00	21.78
20	ATOM	2935	C	THR	B	431	12.603	-11.037	21.480	1.00	21.98
	ATOM	2936	O	THR	B	431	13.595	-10.429	21.879	1.00	19.85
	ATOM	2937	N	SER	B	432	11.844	-11.773	22.280	1.00	24.24
	ATOM	2938	CA	SER	B	432	12.169	-11.906	23.693	1.00	26.96
	ATOM	2939	CB	SER	B	432	11.055	-12.661	24.423	1.00	28.00
25	ATOM	2940	OG	SER	B	432	11.404	-12.888	25.776	1.00	30.31
	ATOM	2941	C	SER	B	432	13.491	-12.660	23.820	1.00	27.67
	ATOM	2942	O	SER	B	432	14.305	-12.377	24.701	1.00	23.78
	ATOM	2943	N	SER	B	433	13.691	-13.628	22.932	1.00	29.27
	ATOM	2944	CA	SER	B	433	14.914	-14.421	22.928	1.00	31.96
30	ATOM	2945	CB	SER	B	433	14.790	-15.575	21.938	1.00	30.84
	ATOM	2946	OG	SER	B	433	14.761	-16.808	22.625	1.00	38.26
	ATOM	2947	C	SER	B	433	16.104	-13.550	22.548	1.00	31.47
	ATOM	2948	O	SER	B	433	17.204	-13.701	23.087	1.00	28.43
	ATOM	2949	N	ARG	B	434	15.878	-12.641	21.607	1.00	29.55
35	ATOM	2950	CA	ARG	B	434	16.926	-11.739	21.165	1.00	29.40
	ATOM	2951	CB	ARG	B	434	16.437	-10.912	19.977	1.00	31.56
	ATOM	2952	CG	ARG	B	434	17.428	-9.868	19.493	1.00	36.76
	ATOM	2953	CD	ARG	B	434	18.694	-10.502	18.919	1.00	37.76
	ATOM	2954	NE	ARG	B	434	19.654	-9.479	18.516	1.00	39.50
40	ATOM	2955	CZ	ARG	B	434	20.965	-9.673	18.418	1.00	44.17
	ATOM	2956	NH1	ARG	B	434	21.492	-10.861	18.696	1.00	43.17
	ATOM	2957	NH2	ARG	B	434	21.750	-8.671	18.048	1.00	43.05
	ATOM	2958	C	ARG	B	434	17.328	-10.827	22.326	1.00	29.15
	ATOM	2959	O	ARG	B	434	18.515	-10.612	22.569	1.00	28.82
45	ATOM	2960	N	PHE	B	435	16.337	-10.297	23.039	1.00	24.88
	ATOM	2961	CA	PHE	B	435	16.600	-9.422	24.186	1.00	25.74
	ATOM	2962	CB	PHE	B	435	15.278	-8.972	24.825	1.00	26.53
	ATOM	2963	CG	PHE	B	435	14.656	-7.758	24.183	1.00	30.94

	ATOM	2964	CD1	PHE	B	435	15.118	-7.271	22.966	1.00	32.65
	ATOM	2965	CD2	PHE	B	435	13.592	-7.108	24.797	1.00	33.60
	ATOM	2966	CE1	PHE	B	435	14.529	-6.155	22.372	1.00	36.84
	ATOM	2967	CE2	PHE	B	435	12.997	-5.989	24.208	1.00	34.96
	ATOM	2968	CZ	PHE	B	435	13.468	-5.516	22.995	1.00	31.64
	ATOM	2969	C	PHE	B	435	17.426	-10.184	25.233	1.00	25.39
	ATOM	2970	O	PHE	B	435	18.414	-9.675	25.764	1.00	22.59
	ATOM	2971	N	ARG	B	436	16.999	-11.405	25.528	1.00	24.58
	ATOM	2972	CA	ARG	B	436	17.675	-12.253	26.503	1.00	30.25
	ATOM	2973	CB	ARG	B	436	16.898	-13.569	26.662	1.00	33.32
	ATOM	2974	CG	ARG	B	436	17.232	-14.358	27.915	1.00	38.17
	ATOM	2975	CD	ARG	B	436	16.135	-15.367	28.260	1.00	37.27
	ATOM	2976	NE	ARG	B	436	15.646	-16.085	27.086	1.00	43.92
	ATOM	2977	CZ	ARG	B	436	14.433	-15.923	26.557	1.00	46.68
	ATOM	2978	NH1	ARG	B	436	13.578	-15.061	27.097	1.00	45.59
	ATOM	2979	NH2	ARG	B	436	14.074	-16.620	25.486	1.00	46.25
	ATOM	2980	C	ARG	B	436	19.110	-12.531	26.048	1.00	29.82
	ATOM	2981	O	ARG	B	436	20.057	-12.397	26.823	1.00	28.76
	ATOM	2982	N	AMET	B	437	19.269	-12.921	24.789	0.50	30.27
	ATOM	2983	N	BMET	B	437	19.252	-12.906	24.781	0.50	31.41
	ATOM	2984	CA	AMET	B	437	20.591	-13.212	24.253	0.50	31.98
	ATOM	2985	CA	BMET	B	437	20.547	-13.206	24.183	0.50	33.77
	ATOM	2986	CB	AMET	B	437	20.489	-13.646	22.788	0.50	31.34
	ATOM	2987	CB	BMET	B	437	20.348	-13.595	22.714	0.50	35.88
	ATOM	2988	CG	AMET	B	437	20.179	-15.127	22.592	0.50	33.62
	ATOM	2989	CG	BMET	B	437	21.605	-13.594	21.861	0.50	40.47
	ATOM	2990	SD	AMET	B	437	20.354	-16.099	24.109	0.50	35.21
	ATOM	2991	SD	BMET	B	437	21.247	-13.937	20.115	0.50	46.79
	ATOM	2992	CE	AMET	B	437	22.155	-16.194	24.259	0.50	33.20
	ATOM	2993	CE	BMET	B	437	21.837	-15.632	19.976	0.50	43.22
	ATOM	2994	C	AMET	B	437	21.498	-11.993	24.366	0.50	33.33
	ATOM	2995	C	BMET	B	437	21.487	-12.005	24.289	0.50	34.45
	ATOM	2996	O	AMET	B	437	22.702	-12.123	24.594	0.50	33.54
	ATOM	2997	O	BMET	B	437	22.699	-12.162	24.438	0.50	34.43
	ATOM	2998	N	MET	B	438	20.913	-10.809	24.215	1.00	32.07
	ATOM	2999	CA	MET	B	438	21.674	-9.560	24.298	1.00	32.48
	ATOM	3000	CB	MET	B	438	20.930	-8.437	23.578	1.00	29.74
	ATOM	3001	CG	MET	B	438	21.161	-8.364	22.093	1.00	36.73
	ATOM	3002	SD	MET	B	438	20.425	-6.849	21.462	1.00	38.21
	ATOM	3003	CE	MET	B	438	21.693	-5.657	21.943	1.00	35.91
	ATOM	3004	C	MET	B	438	21.877	-9.122	25.738	1.00	28.81
	ATOM	3005	O	MET	B	438	22.686	-8.240	26.013	1.00	30.13
	ATOM	3006	N	ASN	B	439	21.120	-9.721	26.646	1.00	27.14
	ATOM	3007	CA	ASN	B	439	21.199	-9.359	28.038	1.00	27.34
	ATOM	3008	CB	ASN	B	439	22.592	-9.524	28.598	1.00	34.85
	ATOM	3009	CG	ASN	B	439	22.624	-9.480	30.080	1.00	38.58
	ATOM	3010	OD1	ASN	B	439	21.584	-9.620	30.724	1.00	42.99
	ATOM	3011	ND2	ASN	B	439	23.801	-9.260	30.666	1.00	41.14

	ATOM	3012	C	ASN	B	439	20.745	-7.903	28.212	1.00	26.24
	ATOM	3013	O	ASN	B	439	21.396	-7.106	28.891	1.00	19.76
	ATOM	3014	N	LEU	B	440	19.625	-7.564	27.573	1.00	24.90
	ATOM	3015	CA	LEU	B	440	19.061	-6.214	27.633	1.00	25.04
5	ATOM	3016	CB	LEU	B	440	17.761	-6.157	26.818	1.00	22.36
	ATOM	3017	CG	LEU	B	440	17.087	-4.786	26.740	1.00	26.33
	ATOM	3018	CD1	LEU	B	440	17.958	-3.843	25.923	1.00	28.33
	ATOM	3019	CD2	LEU	B	440	15.704	-4.914	26.111	1.00	24.81
	ATOM	3020	C	LEU	B	440	18.782	-5.785	29.074	1.00	24.71
10	ATOM	3021	O	LEU	B	440	18.131	-6.504	29.830	1.00	26.96
	ATOM	3022	N	GLN	B	441	19.268	-4.609	29.452	1.00	25.54
	ATOM	3023	CA	GLN	B	441	19.060	-4.099	30.807	1.00	25.82
	ATOM	3024	CB	GLN	B	441	20.250	-3.231	31.234	1.00	30.41
	ATOM	3025	CG	GLN	B	441	21.572	-3.956	31.228	1.00	30.50
15	ATOM	3026	CD	GLN	B	441	21.610	-5.028	32.279	1.00	32.75
	ATOM	3027	OE1	GLN	B	441	21.539	-4.772	33.473	1.00	36.52
	ATOM	3028	NE2	GLN	B	441	21.703	-6.288	31.823	1.00	31.09
	ATOM	3029	C	GLN	B	441	17.789	-3.265	30.883	1.00	26.93
	ATOM	3030	O	GLN	B	441	17.303	-2.768	29.866	1.00	25.40
20	ATOM	3031	N	GLY	B	442	17.266	-3.105	32.096	1.00	24.56
	ATOM	3032	CA	GLY	B	442	16.058	-2.327	32.293	1.00	22.82
	ATOM	3033	C	GLY	B	442	16.217	-0.873	31.885	1.00	24.19
	ATOM	3034	O	GLY	B	442	15.290	-0.279	31.341	1.00	20.21
	ATOM	3035	N	GLU	B	443	17.387	-0.293	32.141	1.00	22.92
25	ATOM	3036	CA	GLU	B	443	17.635	1.102	31.778	1.00	23.33
	ATOM	3037	CB	GLU	B	443	18.960	1.590	32.378	1.00	24.26
	ATOM	3038	CG	GLU	B	443	19.005	1.525	33.895	1.00	32.31
	ATOM	3039	CD	GLU	B	443	19.701	0.270	34.402	1.00	37.68
	ATOM	3040	OE1	GLU	B	443	19.343	-0.841	33.948	1.00	35.23
30	ATOM	3041	OE2	GLU	B	443	20.607	0.394	35.252	1.00	42.47
	ATOM	3042	C	GLU	B	443	17.662	1.278	30.262	1.00	23.08
	ATOM	3043	O	GLU	B	443	17.265	2.328	29.747	1.00	21.80
	ATOM	3044	N	GLU	B	444	18.128	0.253	29.552	1.00	21.16
	ATOM	3045	CA	GLU	B	444	18.182	0.302	28.093	1.00	22.60
35	ATOM	3046	CB	GLU	B	444	19.046	-0.834	27.545	1.00	20.89
	ATOM	3047	CG	GLU	B	444	20.545	-0.617	27.705	1.00	23.24
	ATOM	3048	CD	GLU	B	444	21.340	-1.869	27.393	1.00	22.11
	ATOM	3049	OE1	GLU	B	444	20.817	-2.978	27.629	1.00	20.89
	ATOM	3050	OE2	GLU	B	444	22.488	-1.746	26.914	1.00	25.49
40	ATOM	3051	C	GLU	B	444	16.758	0.155	27.552	1.00	21.06
	ATOM	3052	O	GLU	B	444	16.377	0.822	26.597	1.00	23.73
	ATOM	3053	N	PHE	B	445	15.987	-0.730	28.176	1.00	19.01
	ATOM	3054	CA	PHE	B	445	14.600	-0.969	27.792	1.00	19.44
	ATOM	3055	CB	PHE	B	445	13.989	-2.067	28.675	1.00	18.12
45	ATOM	3056	CG	PHE	B	445	12.483	-2.055	28.709	1.00	18.13
	ATOM	3057	CD1	PHE	B	445	11.746	-2.386	27.575	1.00	18.34
	ATOM	3058	CD2	PHE	B	445	11.802	-1.694	29.872	1.00	16.59
	ATOM	3059	CE1	PHE	B	445	10.346	-2.359	27.592	1.00	17.15

	ATOM	3060	CE2	PHE	B	445	10.406	-1.662	29.903	1.00	21.99
	ATOM	3061	CZ	PHE	B	445	9.674	-1.997	28.755	1.00	16.01
	ATOM	3062	C	PHE	B	445	13.758	0.304	27.888	1.00	15.87
	ATOM	3063	O	PHE	B	445	13.008	0.617	26.966	1.00	20.27
5	ATOM	3064	N	VAL	B	446	13.872	1.044	28.986	1.00	15.90
	ATOM	3065	CA	VAL	B	446	13.074	2.269	29.112	1.00	16.78
	ATOM	3066	CB	VAL	B	446	13.165	2.895	30.531	1.00	18.32
	ATOM	3067	CG1	VAL	B	446	12.574	1.923	31.551	1.00	21.14
	ATOM	3068	CG2	VAL	B	446	14.598	3.251	30.879	1.00	21.04
10	ATOM	3069	C	VAL	B	446	13.450	3.295	28.051	1.00	17.91
	ATOM	3070	O	VAL	B	446	12.596	4.028	27.561	1.00	19.37
	ATOM	3071	N	CYS	B	447	14.723	3.335	27.674	1.00	18.81
	ATOM	3072	CA	CYS	B	447	15.161	4.255	26.635	1.00	17.34
	ATOM	3073	CB	CYS	B	447	16.682	4.224	26.512	1.00	19.33
15	ATOM	3074	SG	CYS	B	447	17.538	5.134	27.798	1.00	23.60
	ATOM	3075	C	CYS	B	447	14.537	3.826	25.301	1.00	18.09
	ATOM	3076	O	CYS	B	447	13.988	4.643	24.563	1.00	17.52
	ATOM	3077	N	LEU	B	448	14.623	2.533	25.006	1.00	15.60
	ATOM	3078	CA	LEU	B	448	14.072	1.994	23.767	1.00	16.67
20	ATOM	3079	CB	LEU	B	448	14.328	0.490	23.684	1.00	14.82
	ATOM	3080	CG	LEU	B	448	15.730	0.009	23.301	1.00	23.57
	ATOM	3081	CD1	LEU	B	448	15.722	-1.522	23.169	1.00	21.61
	ATOM	3082	CD2	LEU	B	448	16.167	0.658	21.986	1.00	18.92
	ATOM	3083	C	LEU	B	448	12.573	2.249	23.652	1.00	15.98
25	ATOM	3084	O	LEU	B	448	12.078	2.633	22.590	1.00	18.91
	ATOM	3085	N	LYS	B	449	11.849	2.037	24.745	1.00	17.94
	ATOM	3086	CA	LYS	B	449	10.405	2.232	24.733	1.00	16.66
	ATOM	3087	CB	LYS	B	449	9.796	1.745	26.047	1.00	16.45
	ATOM	3088	CG	LYS	B	449	8.285	1.861	26.115	1.00	16.12
30	ATOM	3089	CD	LYS	B	449	7.730	0.952	27.193	1.00	19.09
	ATOM	3090	CE	LYS	B	449	8.201	1.380	28.580	1.00	17.04
	ATOM	3091	NZ	LYS	B	449	7.159	1.088	29.593	1.00	17.25
	ATOM	3092	C	LYS	B	449	10.058	3.696	24.486	1.00	18.78
	ATOM	3093	O	LYS	B	449	9.103	3.996	23.769	1.00	14.84
35	ATOM	3094	N	SER	B	450	10.837	4.610	25.059	1.00	14.50
	ATOM	3095	CA	SER	B	450	10.591	6.032	24.849	1.00	17.11
	ATOM	3096	CB	SER	B	450	11.440	6.866	25.815	1.00	21.20
	ATOM	3097	OG	SER	B	450	10.859	6.868	27.108	1.00	30.66
	ATOM	3098	C	SER	B	450	10.921	6.418	23.405	1.00	17.84
40	ATOM	3099	O	SER	B	450	10.279	7.292	22.821	1.00	18.82
	ATOM	3100	N	ILE	B	451	11.926	5.768	22.828	1.00	16.88
	ATOM	3101	CA	ILE	B	451	12.305	6.063	21.450	1.00	17.11
	ATOM	3102	CB	ILE	B	451	13.564	5.268	21.025	1.00	16.69
	ATOM	3103	CG2	ILE	B	451	13.724	5.298	19.505	1.00	19.31
45	ATOM	3104	CG1	ILE	B	451	14.804	5.897	21.676	1.00	18.96
	ATOM	3105	CD1	ILE	B	451	16.083	5.130	21.431	1.00	18.98
	ATOM	3106	C	ILE	B	451	11.142	5.711	20.527	1.00	18.09
	ATOM	3107	O	ILE	B	451	10.820	6.464	19.608	1.00	17.07

ATOM	3108	N	ILE	B	452	10.505	4.571	20.786	1.00	18.13
ATOM	3109	CA	ILE	B	452	9.373	4.137	19.976	1.00	16.77
ATOM	3110	CB	ILE	B	452	8.804	2.775	20.477	1.00	17.40
ATOM	3111	CG2	ILE	B	452	7.464	2.496	19.831	1.00	14.33
ATOM	3112	CG1	ILE	B	452	9.763	1.635	20.107	1.00	15.36
ATOM	3113	CD1	ILE	B	452	9.449	0.323	20.805	1.00	17.76
ATOM	3114	C	ILE	B	452	8.271	5.195	20.024	1.00	17.47
ATOM	3115	O	ILE	B	452	7.733	5.586	18.992	1.00	16.50
ATOM	3116	N	LEU	B	453	7.943	5.665	21.222	1.00	16.06
ATOM	3117	CA	LEU	B	453	6.903	6.680	21.374	1.00	17.17
ATOM	3118	CB	LEU	B	453	6.736	7.061	22.850	1.00	16.23
ATOM	3119	CG	LEU	B	453	5.792	8.228	23.163	1.00	17.60
ATOM	3120	CD1	LEU	B	453	4.388	7.881	22.704	1.00	16.94
ATOM	3121	CD2	LEU	B	453	5.816	8.538	24.667	1.00	17.17
ATOM	3122	C	LEU	B	453	7.198	7.941	20.566	1.00	19.33
ATOM	3123	O	LEU	B	453	6.320	8.458	19.879	1.00	21.37
ATOM	3124	N	LEU	B	454	8.434	8.428	20.636	1.00	17.68
ATOM	3125	CA	LEU	B	454	8.789	9.653	19.933	1.00	20.93
ATOM	3126	CB	LEU	B	454	9.959	10.347	20.653	1.00	24.33
ATOM	3127	CG	LEU	B	454	9.735	10.699	22.130	1.00	26.16
ATOM	3128	CD1	LEU	B	454	11.046	11.170	22.749	1.00	24.82
ATOM	3129	CD2	LEU	B	454	8.658	11.777	22.259	1.00	23.79
ATOM	3130	C	LEU	B	454	9.120	9.494	18.449	1.00	20.75
ATOM	3131	O	LEU	B	454	8.941	10.431	17.673	1.00	21.33
ATOM	3132	N	ASN	B	455	9.566	8.311	18.042	1.00	20.54
ATOM	3133	CA	ASN	B	455	9.951	8.093	16.651	1.00	19.46
ATOM	3134	CB	ASN	B	455	11.147	7.149	16.584	1.00	18.58
ATOM	3135	CG	ASN	B	455	11.576	6.871	15.161	1.00	17.64
ATOM	3136	OD1	ASN	B	455	12.106	7.749	14.496	1.00	18.40
ATOM	3137	ND2	ASN	B	455	11.343	5.648	14.686	1.00	15.06
ATOM	3138	C	ASN	B	455	8.925	7.580	15.655	1.00	22.77
ATOM	3139	O	ASN	B	455	8.790	8.127	14.564	1.00	21.94
ATOM	3140	N	SER	B	456	8.224	6.514	16.023	1.00	25.90
ATOM	3141	CA	SER	B	456	7.260	5.873	15.135	1.00	24.76
ATOM	3142	CB	SER	B	456	6.402	4.894	15.939	1.00	26.91
ATOM	3143	OG	SER	B	456	7.212	3.818	16.390	1.00	26.24
ATOM	3144	C	SER	B	456	6.385	6.774	14.272	1.00	26.52
ATOM	3145	O	SER	B	456	6.323	6.588	13.055	1.00	29.22
ATOM	3146	N	GLY	B	457	5.716	7.750	14.872	1.00	22.07
ATOM	3147	CA	GLY	B	457	4.879	8.627	14.076	1.00	25.19
ATOM	3148	C	GLY	B	457	5.510	9.973	13.765	1.00	28.59
ATOM	3149	O	GLY	B	457	4.851	10.850	13.214	1.00	28.31
ATOM	3150	N	VAL	B	458	6.789	10.130	14.092	1.00	31.65
ATOM	3151	CA	VAL	B	458	7.486	11.396	13.879	1.00	38.50
ATOM	3152	CB	VAL	B	458	8.950	11.310	14.373	1.00	36.24
ATOM	3153	CG1	VAL	B	458	9.827	10.650	13.324	1.00	38.50
ATOM	3154	CG2	VAL	B	458	9.463	12.699	14.701	1.00	39.84
ATOM	3155	C	VAL	B	458	7.483	11.982	12.464	1.00	46.30

ATOM	3156	O	VAL	B	458	7.567	13.201	12.302	1.00	47.67
ATOM	3157	N	TYR	B	459	7.393	11.138	11.442	1.00	50.45
ATOM	3158	CA	TYR	B	459	7.385	11.640	10.069	1.00	57.07
ATOM	3159	CB	TYR	B	459	8.233	10.740	9.170	1.00	57.05
ATOM	3160	CG	TYR	B	459	9.673	10.680	9.611	1.00	59.29
ATOM	3161	CD1	TYR	B	459	10.284	11.786	10.203	1.00	60.93
ATOM	3162	CE1	TYR	B	459	11.591	11.725	10.662	1.00	61.86
ATOM	3163	CD2	TYR	B	459	10.414	9.510	9.486	1.00	59.46
ATOM	3164	CE2	TYR	B	459	11.726	9.439	9.943	1.00	59.67
ATOM	3165	CZ	TYR	B	459	12.305	10.548	10.532	1.00	60.84
ATOM	3166	OH	TYR	B	459	13.593	10.477	11.009	1.00	61.39
ATOM	3167	C	TYR	B	459	5.976	11.753	9.514	1.00	61.22
ATOM	3168	O	TYR	B	459	5.629	12.750	8.874	1.00	62.89
ATOM	3169	N	THR	B	460	5.166	10.730	9.768	1.00	65.15
ATOM	3170	CA	THR	B	460	3.783	10.702	9.309	1.00	67.76
ATOM	3171	CB	THR	B	460	3.178	9.283	9.464	1.00	68.02
ATOM	3172	OG1	THR	B	460	1.890	9.235	8.836	1.00	67.03
ATOM	3173	CG2	THR	B	460	3.040	8.916	10.938	1.00	67.31
ATOM	3174	C	THR	B	460	2.945	11.700	10.107	1.00	70.14
ATOM	3175	O	THR	B	460	1.715	11.641	10.099	1.00	72.35
ATOM	3176	N	PHE	B	461	3.625	12.620	10.788	1.00	72.64
ATOM	3177	CA	PHE	B	461	2.969	13.637	11.607	1.00	75.05
ATOM	3178	CB	PHE	B	461	3.977	14.720	12.012	1.00	75.47
ATOM	3179	CG	PHE	B	461	4.235	14.789	13.492	1.00	74.32
ATOM	3180	CD1	PHE	B	461	3.200	14.609	14.404	1.00	73.98
ATOM	3181	CD2	PHE	B	461	5.517	15.025	13.975	1.00	75.22
ATOM	3182	CE1	PHE	B	461	3.438	14.662	15.775	1.00	74.02
ATOM	3183	CE2	PHE	B	461	5.765	15.080	15.344	1.00	74.50
ATOM	3184	CZ	PHE	B	461	4.722	14.897	16.245	1.00	74.10
ATOM	3185	C	PHE	B	461	1.787	14.286	10.896	1.00	76.78
ATOM	3186	O	PHE	B	461	1.775	14.279	9.645	1.00	77.08
ATOM	3187	CB	GLU	B	470	7.873	23.789	14.718	1.00	80.19
ATOM	3188	C	GLU	B	470	8.958	21.731	15.650	1.00	79.30
ATOM	3189	O	GLU	B	470	9.887	21.518	16.432	1.00	78.21
ATOM	3190	N	GLU	B	470	9.096	22.235	13.227	1.00	80.22
ATOM	3191	CA	GLU	B	470	9.060	22.830	14.595	1.00	80.03
ATOM	3192	N	GLU	B	471	7.823	21.037	15.665	1.00	78.31
ATOM	3193	CA	GLU	B	471	7.596	19.956	16.617	1.00	75.83
ATOM	3194	CB	GLU	B	471	6.118	19.543	16.604	1.00	76.70
ATOM	3195	CG	GLU	B	471	5.742	18.544	15.516	1.00	78.42
ATOM	3196	CD	GLU	B	471	5.062	19.198	14.327	1.00	79.69
ATOM	3197	OE1	GLU	B	471	3.829	19.398	14.378	1.00	80.26
ATOM	3198	OE2	GLU	B	471	5.763	19.511	13.340	1.00	80.72
ATOM	3199	C	GLU	B	471	8.487	18.756	16.292	1.00	73.13
ATOM	3200	O	GLU	B	471	8.897	18.021	17.189	1.00	73.86
ATOM	3201	N	LYS	B	472	8.785	18.565	15.009	1.00	69.65
ATOM	3202	CA	LYS	B	472	9.639	17.461	14.581	1.00	64.40
ATOM	3203	CB	LYS	B	472	9.578	17.293	13.060	1.00	63.78

ATOM	3204	CG	LYS	B	472	8.343	16.552	12.566	1.00	64.49
ATOM	3205	CD	LYS	B	472	8.544	16.002	11.161	1.00	63.81
ATOM	3206	CE	LYS	B	472	7.379	16.368	10.249	1.00	64.90
ATOM	3207	NZ	LYS	B	472	6.475	15.212	9.990	1.00	63.97
ATOM	3208	C	LYS	B	472	11.071	17.749	15.014	1.00	61.03
ATOM	3209	O	LYS	B	472	11.848	16.833	15.287	1.00	60.28
ATOM	3210	N	ASP	B	473	11.413	19.033	15.076	1.00	56.84
ATOM	3211	CA	ASP	B	473	12.745	19.451	15.488	1.00	51.69
ATOM	3212	CB	ASP	B	473	12.923	20.940	15.242	1.00	50.36
ATOM	3213	C	ASP	B	473	12.923	19.138	16.970	1.00	49.18
ATOM	3214	O	ASP	B	473	13.959	18.619	17.385	1.00	46.85
ATOM	3215	N	HIS	B	474	11.898	19.449	17.758	1.00	45.35
ATOM	3216	CA	HIS	B	474	11.923	19.203	19.196	1.00	43.65
ATOM	3217	CB	HIS	B	474	10.652	19.761	19.847	1.00	43.70
ATOM	3218	CG	HIS	B	474	10.458	19.326	21.267	1.00	43.86
ATOM	3219	CD2	HIS	B	474	11.095	19.688	22.406	1.00	44.12
ATOM	3220	ND1	HIS	B	474	9.510	18.395	21.638	1.00	46.60
ATOM	3221	CE1	HIS	B	474	9.572	18.202	22.943	1.00	45.29
ATOM	3222	NE2	HIS	B	474	10.526	18.975	23.434	1.00	47.96
ATOM	3223	C	HIS	B	474	12.030	17.707	19.471	1.00	42.38
ATOM	3224	O	HIS	B	474	12.834	17.273	20.298	1.00	42.83
ATOM	3225	N	ILE	B	475	11.214	16.923	18.773	1.00	38.86
ATOM	3226	CA	ILE	B	475	11.222	15.475	18.943	1.00	36.53
ATOM	3227	CB	ILE	B	475	10.105	14.822	18.110	1.00	36.56
ATOM	3228	CG2	ILE	B	475	10.390	13.335	17.911	1.00	36.17
ATOM	3229	CG1	ILE	B	475	8.770	14.998	18.832	1.00	35.81
ATOM	3230	CD1	ILE	B	475	7.598	14.410	18.094	1.00	41.77
ATOM	3231	C	ILE	B	475	12.575	14.898	18.532	1.00	33.72
ATOM	3232	O	ILE	B	475	13.112	14.023	19.207	1.00	31.50
ATOM	3233	N	HIS	B	476	13.121	15.375	17.429	1.00	33.65
ATOM	3234	CA	HIS	B	476	14.421	14.886	16.992	1.00	33.31
ATOM	3235	CB	HIS	B	476	14.782	15.481	15.637	1.00	37.30
ATOM	3236	CG	HIS	B	476	14.132	14.781	14.486	1.00	43.64
ATOM	3237	CD2	HIS	B	476	13.723	13.498	14.342	1.00	45.25
ATOM	3238	ND1	HIS	B	476	13.816	15.419	13.306	1.00	48.37
ATOM	3239	CE1	HIS	B	476	13.238	14.560	12.484	1.00	48.87
ATOM	3240	NE2	HIS	B	476	13.170	13.387	13.089	1.00	48.11
ATOM	3241	C	HIS	B	476	15.506	15.213	18.022	1.00	31.20
ATOM	3242	O	HIS	B	476	16.442	14.436	18.208	1.00	27.25
ATOM	3243	N	ARG	B	477	15.387	16.365	18.684	1.00	30.64
ATOM	3244	CA	ARG	B	477	16.361	16.754	19.703	1.00	30.09
ATOM	3245	CB	ARG	B	477	16.144	18.214	20.121	1.00	33.46
ATOM	3246	CG	ARG	B	477	16.322	19.212	18.982	1.00	40.74
ATOM	3247	CD	ARG	B	477	16.274	20.649	19.479	1.00	45.91
ATOM	3248	NE	ARG	B	477	17.514	21.020	20.155	1.00	51.37
ATOM	3249	CZ	ARG	B	477	18.375	21.927	19.702	1.00	53.68
ATOM	3250	NH1	ARG	B	477	18.140	22.567	18.560	1.00	53.04
ATOM	3251	NH2	ARG	B	477	19.480	22.185	20.389	1.00	51.79

ATOM	3252	C	ARG	B	477	16.232	15.835	20.925	1.00	26.97
ATOM	3253	O	ARG	B	477	17.233	15.387	21.486	1.00	27.34
ATOM	3254	N	VAL	B	478	14.999	15.558	21.338	1.00	23.70
ATOM	3255	CA	VAL	B	478	14.780	14.685	22.482	1.00	24.79
ATOM	3256	CB	VAL	B	478	13.286	14.613	22.861	1.00	24.83
ATOM	3257	CG1	VAL	B	478	13.088	13.646	24.022	1.00	26.23
ATOM	3258	CG2	VAL	B	478	12.781	15.996	23.243	1.00	28.26
ATOM	3259	C	VAL	B	478	15.284	13.294	22.112	1.00	26.10
ATOM	3260	O	VAL	B	478	15.919	12.613	22.927	1.00	24.28
ATOM	3261	N	LEU	B	479	15.021	12.889	20.870	1.00	22.92
ATOM	3262	CA	LEU	B	479	15.456	11.584	20.379	1.00	21.96
ATOM	3263	CB	LEU	B	479	14.992	11.372	18.930	1.00	22.63
ATOM	3264	CG	LEU	B	479	13.575	10.798	18.756	1.00	20.82
ATOM	3265	CD1	LEU	B	479	13.231	10.689	17.274	1.00	22.53
ATOM	3266	CD2	LEU	B	479	13.495	9.440	19.420	1.00	23.08
ATOM	3267	C	LEU	B	479	16.975	11.471	20.453	1.00	21.90
ATOM	3268	O	LEU	B	479	17.506	10.416	20.778	1.00	23.11
ATOM	3269	N	ASP	B	480	17.675	12.560	20.143	1.00	23.65
ATOM	3270	CA	ASP	B	480	19.141	12.566	20.198	1.00	24.29
ATOM	3271	CB	ASP	B	480	19.692	13.889	19.649	1.00	26.88
ATOM	3272	CG	ASP	B	480	19.773	13.914	18.129	1.00	33.32
ATOM	3273	OD1	ASP	B	480	19.857	12.836	17.499	1.00	35.44
ATOM	3274	OD2	ASP	B	480	19.757	15.022	17.563	1.00	32.44
ATOM	3275	C	ASP	B	480	19.590	12.406	21.656	1.00	24.13
ATOM	3276	O	ASP	B	480	20.551	11.697	21.956	1.00	24.88
ATOM	3277	N	LYS	B	481	18.887	13.077	22.560	1.00	25.18
ATOM	3278	CA	LYS	B	481	19.213	13.010	23.980	1.00	26.78
ATOM	3279	CB	LYS	B	481	18.262	13.898	24.785	1.00	31.37
ATOM	3280	CG	LYS	B	481	18.962	14.788	25.804	1.00	43.84
ATOM	3281	CD	LYS	B	481	18.780	14.260	27.219	1.00	46.08
ATOM	3282	CE	LYS	B	481	20.120	13.928	27.865	1.00	50.99
ATOM	3283	NZ	LYS	B	481	21.177	14.922	27.511	1.00	54.35
ATOM	3284	C	LYS	B	481	19.124	11.575	24.495	1.00	26.87
ATOM	3285	O	LYS	B	481	19.951	11.145	25.305	1.00	20.37
ATOM	3286	N	ILE	B	482	18.124	10.830	24.027	1.00	23.26
ATOM	3287	CA	ILE	B	482	17.981	9.452	24.472	1.00	21.07
ATOM	3288	CB	ILE	B	482	16.655	8.828	24.015	1.00	19.80
ATOM	3289	CG2	ILE	B	482	16.580	7.370	24.491	1.00	17.40
ATOM	3290	CG1	ILE	B	482	15.479	9.606	24.602	1.00	17.16
ATOM	3291	CD1	ILE	B	482	14.136	9.209	23.991	1.00	19.43
ATOM	3292	C	ILE	B	482	19.135	8.616	23.947	1.00	20.21
ATOM	3293	O	ILE	B	482	19.621	7.722	24.640	1.00	25.55
ATOM	3294	N	THR	B	483	19.569	8.896	22.722	1.00	21.89
ATOM	3295	CA	THR	B	483	20.701	8.176	22.141	1.00	22.67
ATOM	3296	CB	THR	B	483	21.030	8.662	20.695	1.00	23.34
ATOM	3297	OG1	THR	B	483	19.890	8.475	19.851	1.00	27.33
ATOM	3298	CG2	THR	B	483	22.203	7.882	20.116	1.00	24.46
ATOM	3299	C	THR	B	483	21.913	8.441	23.035	1.00	23.51

	ATOM	3300	O	THR	B	483	22.650	7.520	23.381	1.00	27.01
	ATOM	3301	N	ASP	B	484	22.119	9.703	23.404	1.00	22.88
	ATOM	3302	CA	ASP	B	484	23.237	10.058	24.276	1.00	24.93
	ATOM	3303	CB	ASP	B	484	23.201	11.546	24.652	1.00	28.69
5	ATOM	3304	CG	ASP	B	484	23.504	12.464	23.485	1.00	29.19
	ATOM	3305	OD1	ASP	B	484	23.982	11.984	22.437	1.00	29.63
	ATOM	3306	OD2	ASP	B	484	23.256	13.681	23.627	1.00	32.02
	ATOM	3307	C	ASP	B	484	23.125	9.249	25.567	1.00	24.40
	ATOM	3308	O	ASP	B	484	24.125	8.780	26.103	1.00	25.60
10	ATOM	3309	N	THR	B	485	21.899	9.096	26.066	1.00	20.16
	ATOM	3310	CA	THR	B	485	21.670	8.365	27.307	1.00	22.28
	ATOM	3311	CB	THR	B	485	20.203	8.521	27.763	1.00	24.64
	ATOM	3312	OG1	THR	B	485	19.878	9.914	27.830	1.00	24.28
	ATOM	3313	CG2	THR	B	485	19.993	7.896	29.133	1.00	23.32
15	ATOM	3314	C	THR	B	485	22.017	6.881	27.188	1.00	22.13
	ATOM	3315	O	THR	B	485	22.574	6.284	28.115	1.00	23.30
	ATOM	3316	N	LEU	B	486	21.686	6.290	26.045	1.00	23.08
	ATOM	3317	CA	LEU	B	486	21.969	4.881	25.792	1.00	22.26
	ATOM	3318	CB	LEU	B	486	21.346	4.452	24.464	1.00	20.93
20	ATOM	3319	CG	LEU	B	486	19.878	4.031	24.533	1.00	24.92
	ATOM	3320	CD1	LEU	B	486	19.295	4.003	23.123	1.00	21.96
	ATOM	3321	CD2	LEU	B	486	19.763	2.658	25.196	1.00	23.90
	ATOM	3322	C	LEU	B	486	23.477	4.634	25.742	1.00	24.12
	ATOM	3323	O	LEU	B	486	23.984	3.681	26.334	1.00	24.02
25	ATOM	3324	N	ILE	B	487	24.191	5.490	25.022	1.00	24.53
	ATOM	3325	CA	ILE	B	487	25.640	5.345	24.913	1.00	25.16
	ATOM	3326	CB	ILE	B	487	26.207	6.379	23.899	1.00	25.57
	ATOM	3327	CG2	ILE	B	487	27.725	6.522	24.051	1.00	24.54
	ATOM	3328	CG1	ILE	B	487	25.857	5.936	22.470	1.00	25.63
30	ATOM	3329	CD1	ILE	B	487	26.538	4.646	22.021	1.00	25.68
	ATOM	3330	C	ILE	B	487	26.275	5.518	26.307	1.00	23.60
	ATOM	3331	O	ILE	B	487	27.200	4.794	26.671	1.00	23.65
	ATOM	3332	N	HIS	B	488	25.755	6.456	27.081	1.00	21.75
	ATOM	3333	CA	HIS	B	488	26.251	6.720	28.431	1.00	26.07
35	ATOM	3334	CB	HIS	B	488	25.450	7.871	29.041	1.00	26.99
	ATOM	3335	CG	HIS	B	488	25.818	8.196	30.455	1.00	33.06
	ATOM	3336	CD2	HIS	B	488	25.245	7.838	31.629	1.00	32.79
	ATOM	3337	ND1	HIS	B	488	26.869	9.025	30.779	1.00	36.45
	ATOM	3338	CE1	HIS	B	488	26.927	9.164	32.091	1.00	35.93
40	ATOM	3339	NE2	HIS	B	488	25.953	8.453	32.630	1.00	33.88
	ATOM	3340	C	HIS	B	488	26.123	5.463	29.292	1.00	26.85
	ATOM	3341	O	HIS	B	488	27.071	5.054	29.967	1.00	28.52
	ATOM	3342	N	LEU	B	489	24.949	4.850	29.266	1.00	28.00
	ATOM	3343	CA	LEU	B	489	24.715	3.642	30.040	1.00	25.94
45	ATOM	3344	CB	LEU	B	489	23.298	3.127	29.788	1.00	27.07
	ATOM	3345	CG	LEU	B	489	22.158	3.909	30.445	1.00	31.71
	ATOM	3346	CD1	LEU	B	489	20.827	3.516	29.799	1.00	28.08
	ATOM	3347	CD2	LEU	B	489	22.143	3.616	31.949	1.00	29.30

ATOM	3348	C	LEU	B	489	25.718	2.561	29.642	1.00	26.84
ATOM	3349	O	LEU	B	489	26.241	1.832	30.486	1.00	20.86
ATOM	3350	N	MET	B	490	25.978	2.453	28.345	1.00	23.82
ATOM	3351	CA	MET	B	490	26.900	1.438	27.857	1.00	26.38
ATOM	3352	CB	MET	B	490	26.775	1.306	26.336	1.00	27.29
ATOM	3353	CG	MET	B	490	25.418	0.776	25.895	1.00	21.68
ATOM	3354	SD	MET	B	490	25.208	0.739	24.106	1.00	26.30
ATOM	3355	CE	MET	B	490	23.461	0.412	24.022	1.00	19.66
ATOM	3356	C	MET	B	490	28.341	1.743	28.247	1.00	26.42
ATOM	3357	O	MET	B	490	29.109	0.833	28.574	1.00	24.76
ATOM	3358	N	ALA	B	491	28.713	3.018	28.207	1.00	26.67
ATOM	3359	CA	ALA	B	491	30.074	3.394	28.577	1.00	30.73
ATOM	3360	CB	ALA	B	491	30.299	4.882	28.335	1.00	26.66
ATOM	3361	C	ALA	B	491	30.250	3.053	30.056	1.00	32.08
ATOM	3362	O	ALA	B	491	31.194	2.361	30.438	1.00	34.66
ATOM	3363	N	LYS	B	492	29.316	3.523	30.878	1.00	33.17
ATOM	3364	CA	LYS	B	492	29.354	3.267	32.309	1.00	32.82
ATOM	3365	CB	LYS	B	492	28.110	3.849	32.976	1.00	36.38
ATOM	3366	CG	LYS	B	492	28.412	4.797	34.123	1.00	38.68
ATOM	3367	CD	LYS	B	492	27.242	4.887	35.084	1.00	41.41
ATOM	3368	CE	LYS	B	492	26.299	6.013	34.698	1.00	47.57
ATOM	3369	NZ	LYS	B	492	26.395	7.184	35.618	1.00	50.76
ATOM	3370	C	LYS	B	492	29.453	1.771	32.619	1.00	34.08
ATOM	3371	O	LYS	B	492	30.090	1.382	33.593	1.00	34.31
ATOM	3372	N	ALA	B	493	28.835	0.935	31.788	1.00	32.03
ATOM	3373	CA	ALA	B	493	28.867	-0.510	31.998	1.00	30.70
ATOM	3374	CB	ALA	B	493	27.719	-1.181	31.245	1.00	28.80
ATOM	3375	C	ALA	B	493	30.201	-1.156	31.606	1.00	33.75
ATOM	3376	O	ALA	B	493	30.402	-2.356	31.819	1.00	30.53
ATOM	3377	N	GLY	B	494	31.102	-0.372	31.020	1.00	33.50
ATOM	3378	CA	GLY	B	494	32.405	-0.903	30.656	1.00	33.71
ATOM	3379	C	GLY	B	494	32.639	-1.360	29.230	1.00	34.40
ATOM	3380	O	GLY	B	494	33.663	-1.989	28.950	1.00	33.13
ATOM	3381	N	LEU	B	495	31.712	-1.056	28.326	1.00	31.76
ATOM	3382	CA	LEU	B	495	31.859	-1.452	26.925	1.00	30.57
ATOM	3383	CB	LEU	B	495	30.494	-1.415	26.216	1.00	30.67
ATOM	3384	CG	LEU	B	495	29.610	-2.675	26.256	1.00	29.59
ATOM	3385	CD1	LEU	B	495	29.315	-3.058	27.700	1.00	26.60
ATOM	3386	CD2	LEU	B	495	28.307	-2.416	25.501	1.00	27.52
ATOM	3387	C	LEU	B	495	32.829	-0.515	26.202	1.00	30.53
ATOM	3388	O	LEU	B	495	32.855	0.688	26.468	1.00	28.14
ATOM	3389	N	THR	B	496	33.628	-1.064	25.291	1.00	28.03
ATOM	3390	CA	THR	B	496	34.567	-0.243	24.529	1.00	29.06
ATOM	3391	CB	THR	B	496	35.511	-1.095	23.665	1.00	29.40
ATOM	3392	OG1	THR	B	496	34.753	-1.758	22.641	1.00	30.29
ATOM	3393	CG2	THR	B	496	36.228	-2.122	24.515	1.00	28.12
ATOM	3394	C	THR	B	496	33.770	0.652	23.590	1.00	30.12
ATOM	3395	O	THR	B	496	32.580	0.433	23.380	1.00	29.74

	ATOM	3396	N	LEU	B	497	34.430	1.654	23.018	1.00	30.44
	ATOM	3397	CA	LEU	B	497	33.762	2.567	22.104	1.00	28.54
	ATOM	3398	CB	LEU	B	497	34.768	3.564	21.529	1.00	31.14
	ATOM	3399	CG	LEU	B	497	35.209	4.719	22.434	1.00	33.58
5	ATOM	3400	CD1	LEU	B	497	36.120	5.659	21.652	1.00	31.42
	ATOM	3401	CD2	LEU	B	497	33.992	5.469	22.942	1.00	35.08
	ATOM	3402	C	LEU	B	497	33.095	1.800	20.967	1.00	27.35
	ATOM	3403	O	LEU	B	497	31.967	2.105	20.574	1.00	24.03
	ATOM	3404	N	GLN	B	498	33.798	0.797	20.447	1.00	26.17
10	ATOM	3405	CA	GLN	B	498	33.289	-0.009	19.348	1.00	26.32
	ATOM	3406	CB	GLN	B	498	34.411	-0.876	18.771	1.00	27.25
	ATOM	3407	CG	GLN	B	498	33.967	-1.796	17.645	1.00	32.67
	ATOM	3408	CD	GLN	B	498	34.965	-2.912	17.374	1.00	38.39
	ATOM	3409	OE1	GLN	B	498	35.737	-3.298	18.254	1.00	36.78
15	ATOM	3410	NE2	GLN	B	498	34.953	-3.437	16.153	1.00	33.18
	ATOM	3411	C	GLN	B	498	32.112	-0.888	19.774	1.00	25.70
	ATOM	3412	O	GLN	B	498	31.167	-1.076	19.009	1.00	25.35
	ATOM	3413	N	GLN	B	499	32.173	-1.434	20.986	1.00	24.01
	ATOM	3414	CA	GLN	B	499	31.093	-2.281	21.487	1.00	25.34
20	ATOM	3415	CB	GLN	B	499	31.501	-2.935	22.815	1.00	28.38
	ATOM	3416	CG	GLN	B	499	32.537	-4.056	22.669	1.00	29.13
	ATOM	3417	CD	GLN	B	499	32.913	-4.687	23.995	1.00	30.80
	ATOM	3418	OE1	GLN	B	499	33.306	-3.997	24.937	1.00	33.62
	ATOM	3419	NE2	GLN	B	499	32.797	-6.004	24.074	1.00	30.64
25	ATOM	3420	C	GLN	B	499	29.842	-1.430	21.693	1.00	25.70
	ATOM	3421	O	GLN	B	499	28.715	-1.910	21.554	1.00	26.22
	ATOM	3422	N	GLN	B	500	30.062	-0.160	22.020	1.00	23.09
	ATOM	3423	CA	GLN	B	500	28.989	0.793	22.256	1.00	23.53
	ATOM	3424	CB	GLN	B	500	29.564	2.107	22.782	1.00	26.17
30	ATOM	3425	CG	GLN	B	500	29.958	2.073	24.252	1.00	27.71
	ATOM	3426	CD	GLN	B	500	30.812	3.262	24.641	1.00	29.32
	ATOM	3427	OE1	GLN	B	500	30.559	4.386	24.207	1.00	28.48
	ATOM	3428	NE2	GLN	B	500	31.831	3.021	25.463	1.00	25.07
	ATOM	3429	C	GLN	B	500	28.151	1.074	21.015	1.00	24.24
35	ATOM	3430	O	GLN	B	500	26.923	0.949	21.053	1.00	24.40
	ATOM	3431	N	HIS	B	501	28.790	1.465	19.915	1.00	23.08
	ATOM	3432	CA	HIS	B	501	28.004	1.739	18.724	1.00	26.92
	ATOM	3433	CB	HIS	B	501	28.791	2.577	17.697	1.00	32.00
	ATOM	3434	CG	HIS	B	501	29.988	1.896	17.105	1.00	36.97
40	ATOM	3435	CD2	HIS	B	501	30.122	0.710	16.465	1.00	40.32
	ATOM	3436	ND1	HIS	B	501	31.224	2.505	17.042	1.00	37.88
	ATOM	3437	CE1	HIS	B	501	32.066	1.724	16.389	1.00	38.81
	ATOM	3438	NE2	HIS	B	501	31.422	0.628	16.028	1.00	41.21
	ATOM	3439	C	HIS	B	501	27.451	0.457	18.123	1.00	25.91
45	ATOM	3440	O	HIS	B	501	26.369	0.457	17.531	1.00	20.13
	ATOM	3441	N	GLN	B	502	28.165	-0.648	18.317	1.00	24.94
	ATOM	3442	CA	GLN	B	502	27.698	-1.926	17.804	1.00	21.88
	ATOM	3443	CB	GLN	B	502	28.785	-2.996	17.953	1.00	24.62

	ATOM	3444	CG	GLN	B	502	29.796	-3.001	16.797	1.00	26.55
	ATOM	3445	CD	GLN	B	502	30.843	-4.109	16.902	1.00	27.06
	ATOM	3446	OE1	GLN	B	502	30.716	-5.033	17.705	1.00	28.49
	ATOM	3447	NE2	GLN	B	502	31.882	-4.018	16.078	1.00	21.90
5	ATOM	3448	C	GLN	B	502	26.428	-2.341	18.554	1.00	22.39
	ATOM	3449	O	GLN	B	502	25.464	-2.807	17.944	1.00	22.24
	ATOM	3450	N	ARG	B	503	26.421	-2.159	19.874	1.00	20.54
	ATOM	3451	CA	ARG	B	503	25.259	-2.523	20.678	1.00	22.04
	ATOM	3452	CB	ARG	B	503	25.602	-2.519	22.180	1.00	22.51
10	ATOM	3453	CG	ARG	B	503	24.451	-3.022	23.077	1.00	23.34
	ATOM	3454	CD	ARG	B	503	24.853	-3.110	24.550	1.00	22.18
	ATOM	3455	NE	ARG	B	503	23.743	-3.546	25.395	1.00	19.62
	ATOM	3456	CZ	ARG	B	503	23.329	-4.807	25.497	1.00	19.88
	ATOM	3457	NH1	ARG	B	503	23.933	-5.765	24.809	1.00	16.40
15	ATOM	3458	NH2	ARG	B	503	22.303	-5.110	26.280	1.00	19.71
	ATOM	3459	C	ARG	B	503	24.102	-1.558	20.409	1.00	19.05
	ATOM	3460	O	ARG	B	503	22.945	-1.968	20.351	1.00	18.87
	ATOM	3461	N	LEU	B	504	24.414	-0.276	20.239	1.00	20.19
	ATOM	3462	CA	LEU	B	504	23.375	0.714	19.969	1.00	19.33
20	ATOM	3463	CB	LEU	B	504	23.972	2.117	19.855	1.00	16.25
	ATOM	3464	CG	LEU	B	504	22.983	3.173	19.344	1.00	20.35
	ATOM	3465	CD1	LEU	B	504	21.930	3.449	20.427	1.00	17.97
	ATOM	3466	CD2	LEU	B	504	23.729	4.448	18.955	1.00	20.86
	ATOM	3467	C	LEU	B	504	22.659	0.357	18.667	1.00	21.22
25	ATOM	3468	O	LEU	B	504	21.433	0.478	18.566	1.00	19.28
	ATOM	3469	N	ALA	B	505	23.428	-0.085	17.676	1.00	18.55
	ATOM	3470	CA	ALA	B	505	22.859	-0.473	16.396	1.00	18.20
	ATOM	3471	CB	ALA	B	505	23.973	-0.745	15.382	1.00	18.45
	ATOM	3472	C	ALA	B	505	21.986	-1.716	16.562	1.00	19.54
30	ATOM	3473	O	ALA	B	505	20.871	-1.774	16.041	1.00	17.63
	ATOM	3474	N	GLN	B	506	22.497	-2.706	17.293	1.00	20.30
	ATOM	3475	CA	GLN	B	506	21.772	-3.955	17.513	1.00	19.48
	ATOM	3476	CB	GLN	B	506	22.590	-4.893	18.409	1.00	21.75
	ATOM	3477	CG	GLN	B	506	23.798	-5.551	17.727	1.00	20.85
35	ATOM	3478	CD	GLN	B	506	24.819	-6.070	18.736	1.00	26.18
	ATOM	3479	OE1	GLN	B	506	24.564	-6.084	19.943	1.00	21.83
	ATOM	3480	NE2	GLN	B	506	25.977	-6.499	18.245	1.00	25.39
	ATOM	3481	C	GLN	B	506	20.421	-3.672	18.166	1.00	21.39
	ATOM	3482	O	GLN	B	506	19.396	-4.233	17.766	1.00	20.87
40	ATOM	3483	N	LEU	B	507	20.433	-2.800	19.171	1.00	19.52
	ATOM	3484	CA	LEU	B	507	19.219	-2.418	19.884	1.00	23.04
	ATOM	3485	CB	LEU	B	507	19.548	-1.455	21.030	1.00	22.82
	ATOM	3486	CG	LEU	B	507	20.182	-2.011	22.313	1.00	26.12
	ATOM	3487	CD1	LEU	B	507	20.203	-0.916	23.360	1.00	29.33
45	ATOM	3488	CD2	LEU	B	507	19.415	-3.213	22.816	1.00	27.80
	ATOM	3489	C	LEU	B	507	18.212	-1.730	18.971	1.00	22.19
	ATOM	3490	O	LEU	B	507	17.036	-2.070	18.964	1.00	23.00
	ATOM	3491	N	LEU	B	508	18.678	-0.745	18.214	1.00	21.53

	ATOM	3492	CA	LEU	B	508	17.797	0.006	17.332	1.00	20.60
	ATOM	3493	CB	LEU	B	508	18.535	1.236	16.805	1.00	17.57
	ATOM	3494	CG	LEU	B	508	18.934	2.218	17.913	1.00	17.67
	ATOM	3495	CD1	LEU	B	508	19.566	3.446	17.301	1.00	20.04
	ATOM	3496	CD2	LEU	B	508	17.724	2.611	18.725	1.00	18.49
	ATOM	3497	C	LEU	B	508	17.235	-0.831	16.183	1.00	21.17
	ATOM	3498	O	LEU	B	508	16.118	-0.597	15.728	1.00	21.88
	ATOM	3499	N	LEU	B	509	18.000	-1.813	15.713	1.00	21.89
	ATOM	3500	CA	LEU	B	509	17.511	-2.657	14.631	1.00	22.81
	ATOM	3501	CB	LEU	B	509	18.603	-3.597	14.145	1.00	22.65
	ATOM	3502	CG	LEU	B	509	19.645	-2.891	13.278	1.00	29.11
	ATOM	3503	CD1	LEU	B	509	20.697	-3.888	12.829	1.00	25.69
	ATOM	3504	CD2	LEU	B	509	18.965	-2.248	12.082	1.00	27.92
	ATOM	3505	C	LEU	B	509	16.302	-3.462	15.095	1.00	23.32
	ATOM	3506	O	LEU	B	509	15.409	-3.759	14.303	1.00	23.36
	ATOM	3507	N	ILE	B	510	16.264	-3.796	16.380	1.00	23.36
	ATOM	3508	CA	ILE	B	510	15.148	-4.562	16.912	1.00	20.99
	ATOM	3509	CB	ILE	B	510	15.448	-5.041	18.361	1.00	28.60
	ATOM	3510	CG2	ILE	B	510	14.162	-5.435	19.075	1.00	28.10
	ATOM	3511	CG1	ILE	B	510	16.383	-6.260	18.308	1.00	26.57
	ATOM	3512	CD1	ILE	B	510	17.429	-6.301	19.419	1.00	30.14
	ATOM	3513	C	ILE	B	510	13.852	-3.746	16.846	1.00	17.65
	ATOM	3514	O	ILE	B	510	12.767	-4.308	16.759	1.00	16.11
	ATOM	3515	N	LEU	B	511	13.961	-2.421	16.867	1.00	18.12
	ATOM	3516	CA	LEU	B	511	12.772	-1.574	16.774	1.00	16.95
	ATOM	3517	CB	LEU	B	511	13.147	-0.100	16.981	1.00	22.66
	ATOM	3518	CG	LEU	B	511	13.607	0.262	18.406	1.00	22.13
	ATOM	3519	CD1	LEU	B	511	13.404	1.751	18.652	1.00	25.29
	ATOM	3520	CD2	LEU	B	511	12.830	-0.549	19.425	1.00	25.08
	ATOM	3521	C	LEU	B	511	12.112	-1.771	15.397	1.00	16.65
	ATOM	3522	O	LEU	B	511	10.915	-1.578	15.242	1.00	17.09
	ATOM	3523	N	SER	B	512	12.901	-2.161	14.401	1.00	15.83
	ATOM	3524	CA	SER	B	512	12.355	-2.408	13.072	1.00	18.66
	ATOM	3525	CB	SER	B	512	13.484	-2.644	12.074	1.00	17.62
	ATOM	3526	OG	SER	B	512	13.079	-3.550	11.062	1.00	32.77
	ATOM	3527	C	SER	B	512	11.454	-3.638	13.154	1.00	18.54
	ATOM	3528	O	SER	B	512	10.373	-3.683	12.545	1.00	17.01
	ATOM	3529	N	HIS	B	513	11.899	-4.625	13.929	1.00	15.54
	ATOM	3530	CA	HIS	B	513	11.141	-5.860	14.115	1.00	17.67
	ATOM	3531	CB	HIS	B	513	12.013	-6.916	14.790	1.00	19.03
	ATOM	3532	CG	HIS	B	513	13.063	-7.475	13.886	1.00	27.06
	ATOM	3533	CD2	HIS	B	513	12.980	-8.364	12.868	1.00	28.40
	ATOM	3534	ND1	HIS	B	513	14.378	-7.066	13.932	1.00	28.92
	ATOM	3535	CE1	HIS	B	513	15.061	-7.678	12.981	1.00	30.75
	ATOM	3536	NE2	HIS	B	513	14.235	-8.472	12.321	1.00	30.08
	ATOM	3537	C	HIS	B	513	9.895	-5.602	14.958	1.00	15.35
	ATOM	3538	O	HIS	B	513	8.846	-6.192	14.704	1.00	14.83
	ATOM	3539	N	ILE	B	514	10.012	-4.744	15.942	1.00	13.35

ATOM	3540	CA	ILE	B	514	8.865	-4.417	16.776	1.00	15.48
ATOM	3541	CB	ILE	B	514	9.295	-3.534	17.967	1.00	20.02
ATOM	3542	CG2	ILE	B	514	8.067	-2.918	18.650	1.00	12.84
ATOM	3543	CG1	ILE	B	514	10.093	-4.397	18.962	1.00	22.87
ATOM	3544	CD1	ILE	B	514	10.691	-3.641	20.115	1.00	29.62
ATOM	3545	C	ILE	B	514	7.797	-3.717	15.923	1.00	15.16
ATOM	3546	O	ILE	B	514	6.606	-3.972	16.078	1.00	16.61
ATOM	3547	N	ARG	B	515	8.224	-2.823	15.030	1.00	16.33
ATOM	3548	CA	ARG	B	515	7.280	-2.138	14.150	1.00	17.54
ATOM	3549	CB	ARG	B	515	8.010	-1.173	13.214	1.00	20.15
ATOM	3550	CG	ARG	B	515	7.080	-0.454	12.234	1.00	21.47
ATOM	3551	CD	ARG	B	515	6.407	0.749	12.891	1.00	26.05
ATOM	3552	NE	ARG	B	515	7.220	1.948	12.716	1.00	24.91
ATOM	3553	CZ	ARG	B	515	6.734	3.175	12.547	1.00	24.61
ATOM	3554	NH1	ARG	B	515	5.424	3.393	12.522	1.00	22.46
ATOM	3555	NH2	ARG	B	515	7.569	4.182	12.374	1.00	23.15
ATOM	3556	C	ARG	B	515	6.545	-3.182	13.304	1.00	16.60
ATOM	3557	O	ARG	B	515	5.332	-3.093	13.087	1.00	14.51
ATOM	3558	N	HIS	B	516	7.298	-4.171	12.827	1.00	18.50
ATOM	3559	CA	HIS	B	516	6.743	-5.237	11.997	1.00	17.26
ATOM	3560	CB	HIS	B	516	7.861	-6.176	11.533	1.00	18.14
ATOM	3561	CG	HIS	B	516	7.405	-7.223	10.568	1.00	24.87
ATOM	3562	CD2	HIS	B	516	7.060	-8.521	10.754	1.00	26.64
ATOM	3563	ND1	HIS	B	516	7.258	-6.978	9.220	1.00	21.82
ATOM	3564	CE1	HIS	B	516	6.839	-8.078	8.619	1.00	28.42
ATOM	3565	NE2	HIS	B	516	6.711	-9.028	9.526	1.00	24.47
ATOM	3566	C	HIS	B	516	5.685	-6.028	12.759	1.00	16.87
ATOM	3567	O	HIS	B	516	4.596	-6.303	12.240	1.00	14.81
ATOM	3568	N	MET	B	517	5.999	-6.396	13.997	1.00	16.48
ATOM	3569	CA	MET	B	517	5.049	-7.162	14.801	1.00	15.39
ATOM	3570	CB	MET	B	517	5.701	-7.587	16.114	1.00	21.05
ATOM	3571	CG	MET	B	517	6.790	-8.638	15.917	1.00	20.76
ATOM	3572	SD	MET	B	517	7.380	-9.320	17.470	1.00	23.96
ATOM	3573	CE	MET	B	517	8.104	-7.879	18.226	1.00	20.45
ATOM	3574	C	MET	B	517	3.789	-6.368	15.080	1.00	16.23
ATOM	3575	O	MET	B	517	2.688	-6.924	15.148	1.00	16.02
ATOM	3576	N	SER	B	518	3.954	-5.060	15.247	1.00	13.32
ATOM	3577	CA	SER	B	518	2.827	-4.186	15.505	1.00	16.34
ATOM	3578	CB	SER	B	518	3.316	-2.765	15.835	1.00	17.48
ATOM	3579	OG	SER	B	518	2.234	-1.840	15.843	1.00	17.46
ATOM	3580	C	SER	B	518	1.906	-4.147	14.284	1.00	14.73
ATOM	3581	O	SER	B	518	0.688	-4.247	14.417	1.00	19.16
ATOM	3582	N	ASN	B	519	2.474	-4.006	13.091	1.00	14.52
ATOM	3583	CA	ASN	B	519	1.622	-3.953	11.907	1.00	15.35
ATOM	3584	CB	ASN	B	519	2.432	-3.509	10.698	1.00	19.21
ATOM	3585	CG	ASN	B	519	2.700	-2.029	10.729	1.00	20.58
ATOM	3586	OD1	ASN	B	519	1.839	-1.258	11.150	1.00	26.36
ATOM	3587	ND2	ASN	B	519	3.891	-1.618	10.307	1.00	19.62

	ATOM	3588	C	ASN	B	519	0.911	-5.280	11.658	1.00	16.74
	ATOM	3589	O	ASN	B	519	-0.265	-5.299	11.297	1.00	20.58
	ATOM	3590	N	LYS	B	520	1.608	-6.387	11.885	1.00	18.60
	ATOM	3591	CA	LYS	B	520	0.992	-7.699	11.717	1.00	20.04
	ATOM	3592	CB	LYS	B	520	2.038	-8.801	11.872	1.00	25.44
	ATOM	3593	CG	LYS	B	520	3.037	-8.849	10.728	1.00	31.68
	ATOM	3594	CD	LYS	B	520	2.507	-9.663	9.558	1.00	42.56
	ATOM	3595	CE	LYS	B	520	2.186	-8.778	8.364	1.00	45.61
	ATOM	3596	NZ	LYS	B	520	1.435	-9.526	7.312	1.00	46.00
	ATOM	3597	C	LYS	B	520	-0.099	-7.868	12.769	1.00	18.88
	ATOM	3598	O	LYS	B	520	-1.183	-8.358	12.478	1.00	21.75
	ATOM	3599	N	GLY	B	521	0.191	-7.455	13.998	1.00	17.83
	ATOM	3600	CA	GLY	B	521	-0.792	-7.569	15.058	1.00	16.19
	ATOM	3601	C	GLY	B	521	-2.000	-6.674	14.833	1.00	16.59
	ATOM	3602	O	GLY	B	521	-3.128	-7.060	15.125	1.00	16.57
	ATOM	3603	N	MET	B	522	-1.766	-5.467	14.326	1.00	17.48
	ATOM	3604	CA	MET	B	522	-2.852	-4.527	14.042	1.00	18.25
	ATOM	3605	CB	MET	B	522	-2.276	-3.212	13.516	1.00	21.27
	ATOM	3606	CG	MET	B	522	-3.190	-2.018	13.707	1.00	26.97
	ATOM	3607	SD	MET	B	522	-3.199	-1.477	15.417	1.00	30.35
	ATOM	3608	CE	MET	B	522	-1.659	-0.605	15.475	1.00	29.86
	ATOM	3609	C	MET	B	522	-3.794	-5.119	12.989	1.00	18.68
	ATOM	3610	O	MET	B	522	-5.022	-5.008	13.097	1.00	18.80
	ATOM	3611	N	GLU	B	523	-3.205	-5.731	11.966	1.00	18.22
	ATOM	3612	CA	GLU	B	523	-3.968	-6.357	10.889	1.00	23.41
	ATOM	3613	CB	GLU	B	523	-3.031	-6.946	9.830	1.00	28.74
	ATOM	3614	CG	GLU	B	523	-2.224	-5.935	9.030	1.00	34.42
	ATOM	3615	CD	GLU	B	523	-1.095	-6.597	8.239	1.00	45.58
	ATOM	3616	OE1	GLU	B	523	-0.131	-5.894	7.857	1.00	49.48
	ATOM	3617	OE2	GLU	B	523	-1.169	-7.825	7.999	1.00	45.97
	ATOM	3618	C	GLU	B	523	-4.812	-7.482	11.465	1.00	23.98
	ATOM	3619	O	GLU	B	523	-5.993	-7.616	11.147	1.00	22.08
	ATOM	3620	N	HIS	B	524	-4.187	-8.287	12.326	1.00	23.46
	ATOM	3621	CA	HIS	B	524	-4.846	-9.428	12.952	1.00	26.20
	ATOM	3622	CB	HIS	B	524	-3.824	-10.245	13.743	1.00	27.26
	ATOM	3623	CG	HIS	B	524	-4.378	-11.509	14.321	1.00	30.91
	ATOM	3624	CD2	HIS	B	524	-4.308	-12.792	13.892	1.00	30.90
	ATOM	3625	ND1	HIS	B	524	-5.107	-11.537	15.490	1.00	28.87
	ATOM	3626	CE1	HIS	B	524	-5.461	-12.780	15.757	1.00	30.45
	ATOM	3627	NE2	HIS	B	524	-4.989	-13.561	14.803	1.00	29.19
	ATOM	3628	C	HIS	B	524	-5.996	-9.025	13.870	1.00	27.69
	ATOM	3629	O	HIS	B	524	-7.061	-9.656	13.860	1.00	25.00
	ATOM	3630	N	LEU	B	525	-5.777	-7.977	14.655	1.00	23.84
	ATOM	3631	CA	LEU	B	525	-6.786	-7.492	15.588	1.00	25.77
	ATOM	3632	CB	LEU	B	525	-6.217	-6.358	16.444	1.00	22.22
	ATOM	3633	CG	LEU	B	525	-7.164	-5.778	17.498	1.00	26.81
	ATOM	3634	CD1	LEU	B	525	-7.763	-6.922	18.321	1.00	23.32
	ATOM	3635	CD2	LEU	B	525	-6.414	-4.793	18.399	1.00	18.95

ATOM	3636	C	LEU	B	525	-8.013	-6.995	14.842	1.00	26.84
ATOM	3637	O	LEU	B	525	-9.154	-7.247	15.249	1.00	26.73
ATOM	3638	N	TYR	B	526	-7.764	-6.271	13.757	1.00	26.86
ATOM	3639	CA	TYR	B	526	-8.819	-5.726	12.918	1.00	30.89
ATOM	3640	CB	TYR	B	526	-8.201	-4.818	11.854	1.00	34.31
ATOM	3641	CG	TYR	B	526	-9.183	-4.223	10.878	1.00	43.50
ATOM	3642	CD1	TYR	B	526	-10.058	-3.211	11.267	1.00	47.66
ATOM	3643	CE1	TYR	B	526	-10.943	-2.636	10.357	1.00	48.85
ATOM	3644	CD2	TYR	B	526	-9.218	-4.651	9.552	1.00	48.52
ATOM	3645	CE2	TYR	B	526	-10.098	-4.083	8.634	1.00	52.43
ATOM	3646	CZ	TYR	B	526	-10.955	-3.077	9.043	1.00	51.67
ATOM	3647	OH	TYR	B	526	-11.810	-2.504	8.129	1.00	57.01
ATOM	3648	C	TYR	B	526	-9.577	-6.880	12.265	1.00	30.90
ATOM	3649	O	TYR	B	526	-10.793	-6.829	12.113	1.00	31.48
ATOM	3650	N	SER	B	527	-8.849	-7.926	11.889	1.00	31.39
ATOM	3651	CA	SER	B	527	-9.460	-9.095	11.266	1.00	33.73
ATOM	3652	CB	SER	B	527	-8.377	-10.048	10.749	1.00	34.13
ATOM	3653	OG	SER	B	527	-8.945	-11.222	10.196	1.00	43.67
ATOM	3654	C	SER	B	527	-10.339	-9.813	12.288	1.00	34.34
ATOM	3655	O	SER	B	527	-11.446	-10.261	11.973	1.00	33.42
ATOM	3656	N	MET	B	528	-9.840	-9.916	13.517	1.00	31.66
ATOM	3657	CA	MET	B	528	-10.574	-10.572	14.589	1.00	29.77
ATOM	3658	CB	MET	B	528	-9.682	-10.743	15.820	1.00	32.96
ATOM	3659	CG	MET	B	528	-8.651	-11.859	15.699	1.00	33.47
ATOM	3660	SD	MET	B	528	-9.359	-13.427	15.134	1.00	38.28
ATOM	3661	CE	MET	B	528	-10.265	-13.915	16.579	1.00	36.01
ATOM	3662	C	MET	B	528	-11.800	-9.747	14.953	1.00	29.42
ATOM	3663	O	MET	B	528	-12.835	-10.293	15.331	1.00	28.65
ATOM	3664	N	LYS	B	529	-11.673	-8.429	14.850	1.00	30.64
ATOM	3665	CA	LYS	B	529	-12.781	-7.533	15.149	1.00	31.80
ATOM	3666	CB	LYS	B	529	-12.323	-6.079	15.027	1.00	32.86
ATOM	3667	CG	LYS	B	529	-13.436	-5.043	15.114	1.00	36.42
ATOM	3668	CD	LYS	B	529	-13.114	-3.852	14.224	1.00	41.74
ATOM	3669	CE	LYS	B	529	-13.734	-2.564	14.741	1.00	43.45
ATOM	3670	NZ	LYS	B	529	-15.221	-2.569	14.634	1.00	46.51
ATOM	3671	C	LYS	B	529	-13.857	-7.840	14.116	1.00	36.60
ATOM	3672	O	LYS	B	529	-15.049	-7.877	14.424	1.00	34.04
ATOM	3673	N	CYS	B	530	-13.407	-8.083	12.889	1.00	40.04
ATOM	3674	CA	CYS	B	530	-14.286	-8.409	11.773	1.00	44.58
ATOM	3675	CB	CYS	B	530	-13.460	-8.535	10.491	1.00	50.64
ATOM	3676	SG	CYS	B	530	-13.369	-7.034	9.504	1.00	67.65
ATOM	3677	C	CYS	B	530	-15.065	-9.692	12.016	1.00	42.88
ATOM	3678	O	CYS	B	530	-16.274	-9.741	11.807	1.00	40.15
ATOM	3679	N	LYS	B	531	-14.360	-10.733	12.447	1.00	41.92
ATOM	3680	CA	LYS	B	531	-14.980	-12.023	12.728	1.00	42.60
ATOM	3681	CB	LYS	B	531	-13.907	-13.091	12.927	1.00	44.77
ATOM	3682	C	LYS	B	531	-15.844	-11.907	13.977	1.00	44.43
ATOM	3683	O	LYS	B	531	-16.623	-12.804	14.296	1.00	44.09

ATOM	3684	N	ASN	B	532	-15.678	-10.793	14.685	1.00	44.98
ATOM	3685	CA	ASN	B	532	-16.437	-10.496	15.893	1.00	44.10
ATOM	3686	CB	ASN	B	532	-17.833	-10.003	15.506	1.00	45.14
ATOM	3687	CG	ASN	B	532	-18.526	-9.271	16.633	1.00	46.54
ATOM	3688	OD1	ASN	B	532	-19.729	-9.424	16.837	1.00	50.62
ATOM	3689	ND2	ASN	B	532	-17.771	-8.471	17.375	1.00	46.07
ATOM	3690	C	ASN	B	532	-16.557	-11.657	16.882	1.00	43.34
ATOM	3691	O	ASN	B	532	-17.655	-11.994	17.321	1.00	41.42
ATOM	3692	N	VAL	B	533	-15.434	-12.264	17.243	1.00	43.45
ATOM	3693	CA	VAL	B	533	-15.471	-13.371	18.190	1.00	44.06
ATOM	3694	CB	VAL	B	533	-14.170	-14.219	18.120	1.00	45.56
ATOM	3695	CG1	VAL	B	533	-13.661	-14.263	16.683	1.00	45.67
ATOM	3696	CG2	VAL	B	533	-13.107	-13.644	19.045	1.00	44.16
ATOM	3697	C	VAL	B	533	-15.670	-12.835	19.611	1.00	43.24
ATOM	3698	O	VAL	B	533	-15.894	-13.602	20.548	1.00	44.21
ATOM	3699	N	VAL	B	534	-15.596	-11.511	19.755	1.00	40.44
ATOM	3700	CA	VAL	B	534	-15.765	-10.849	21.049	1.00	37.80
ATOM	3701	CB	VAL	B	534	-14.630	-11.259	22.038	1.00	36.38
ATOM	3702	CG1	VAL	B	534	-13.324	-10.575	21.658	1.00	34.35
ATOM	3703	CG2	VAL	B	534	-15.021	-10.910	23.463	1.00	39.34
ATOM	3704	C	VAL	B	534	-15.752	-9.329	20.857	1.00	37.97
ATOM	3705	O	VAL	B	534	-15.026	-8.808	20.008	1.00	39.45
ATOM	3706	N	PRO	B	535	-16.575	-8.597	21.625	1.00	37.81
ATOM	3707	CD	PRO	B	535	-17.529	-9.078	22.640	1.00	38.74
ATOM	3708	CA	PRO	B	535	-16.608	-7.135	21.492	1.00	36.79
ATOM	3709	CB	PRO	B	535	-17.846	-6.729	22.288	1.00	36.98
ATOM	3710	CG	PRO	B	535	-18.004	-7.809	23.298	1.00	39.77
ATOM	3711	C	PRO	B	535	-15.338	-6.494	22.049	1.00	33.95
ATOM	3712	O	PRO	B	535	-14.786	-6.963	23.040	1.00	34.93
ATOM	3713	N	LEU	B	536	-14.881	-5.426	21.409	1.00	33.42
ATOM	3714	CA	LEU	B	536	-13.675	-4.732	21.851	1.00	33.40
ATOM	3715	CB	LEU	B	536	-12.829	-4.314	20.647	1.00	29.31
ATOM	3716	CG	LEU	B	536	-12.219	-5.433	19.798	1.00	30.06
ATOM	3717	CD1	LEU	B	536	-11.344	-4.822	18.714	1.00	30.85
ATOM	3718	CD2	LEU	B	536	-11.398	-6.370	20.676	1.00	28.96
ATOM	3719	C	LEU	B	536	-14.036	-3.498	22.666	1.00	30.50
ATOM	3720	O	LEU	B	536	-15.024	-2.829	22.383	1.00	29.91
ATOM	3721	N	TYR	B	537	-13.231	-3.194	23.676	1.00	28.69
ATOM	3722	CA	TYR	B	537	-13.494	-2.032	24.505	1.00	29.89
ATOM	3723	CB	TYR	B	537	-12.618	-2.071	25.750	1.00	32.50
ATOM	3724	CG	TYR	B	537	-12.849	-3.327	26.543	1.00	39.46
ATOM	3725	CD1	TYR	B	537	-13.923	-3.431	27.421	1.00	41.90
ATOM	3726	CE1	TYR	B	537	-14.174	-4.609	28.118	1.00	45.72
ATOM	3727	CD2	TYR	B	537	-12.022	-4.435	26.379	1.00	47.39
ATOM	3728	CE2	TYR	B	537	-12.262	-5.620	27.072	1.00	49.93
ATOM	3729	CZ	TYR	B	537	-13.340	-5.699	27.940	1.00	48.80
ATOM	3730	OH	TYR	B	537	-13.582	-6.872	28.624	1.00	53.90
ATOM	3731	C	TYR	B	537	-13.262	-0.761	23.709	1.00	27.09

ATOM	3732	O	TYR	B	537	-12.518	-0.757	22.729	1.00	26.15
ATOM	3733	N	ASP	B	538	-13.909	0.315	24.141	1.00	26.12
ATOM	3734	CA	ASP	B	538	-13.830	1.598	23.461	1.00	25.27
ATOM	3735	CB	ASP	B	538	-14.748	2.598	24.164	1.00	28.85
ATOM	3736	CG	ASP	B	538	-16.227	2.285	23.940	1.00	33.90
ATOM	3737	OD1	ASP	B	538	-17.052	2.613	24.819	1.00	32.68
ATOM	3738	OD2	ASP	B	538	-16.562	1.707	22.882	1.00	38.26
ATOM	3739	C	ASP	B	538	-12.447	2.217	23.261	1.00	25.18
ATOM	3740	O	ASP	B	538	-12.120	2.626	22.147	1.00	26.41
ATOM	3741	N	LEU	B	539	-11.637	2.309	24.313	1.00	20.76
ATOM	3742	CA	LEU	B	539	-10.312	2.911	24.150	1.00	19.65
ATOM	3743	CB	LEU	B	539	-9.567	2.991	25.496	1.00	17.48
ATOM	3744	CG	LEU	B	539	-8.116	3.511	25.469	1.00	16.46
ATOM	3745	CD1	LEU	B	539	-8.051	4.892	24.838	1.00	16.43
ATOM	3746	CD2	LEU	B	539	-7.564	3.569	26.895	1.00	15.57
ATOM	3747	C	LEU	B	539	-9.484	2.127	23.127	1.00	16.75
ATOM	3748	O	LEU	B	539	-8.862	2.716	22.249	1.00	20.36
ATOM	3749	N	LEU	B	540	-9.487	0.803	23.239	1.00	18.23
ATOM	3750	CA	LEU	B	540	-8.743	-0.048	22.319	1.00	18.05
ATOM	3751	CB	LEU	B	540	-8.909	-1.528	22.701	1.00	16.38
ATOM	3752	CG	LEU	B	540	-8.188	-2.554	21.821	1.00	19.81
ATOM	3753	CD1	LEU	B	540	-6.679	-2.303	21.828	1.00	19.27
ATOM	3754	CD2	LEU	B	540	-8.473	-3.952	22.327	1.00	18.00
ATOM	3755	C	LEU	B	540	-9.241	0.169	20.891	1.00	21.50
ATOM	3756	O	LEU	B	540	-8.449	0.293	19.964	1.00	20.41
ATOM	3757	N	LEU	B	541	-10.559	0.206	20.726	1.00	22.40
ATOM	3758	CA	LEU	B	541	-11.164	0.419	19.413	1.00	23.27
ATOM	3759	CB	LEU	B	541	-12.686	0.429	19.527	1.00	25.12
ATOM	3760	CG	LEU	B	541	-13.410	-0.808	18.999	1.00	36.53
ATOM	3761	CD1	LEU	B	541	-14.910	-0.671	19.273	1.00	30.98
ATOM	3762	CD2	LEU	B	541	-13.136	-0.971	17.508	1.00	31.93
ATOM	3763	C	LEU	B	541	-10.697	1.751	18.842	1.00	22.46
ATOM	3764	O	LEU	B	541	-10.359	1.845	17.666	1.00	26.29
ATOM	3765	N	GLU	B	542	-10.694	2.781	19.680	1.00	23.96
ATOM	3766	CA	GLU	B	542	-10.248	4.106	19.270	1.00	26.91
ATOM	3767	CB	GLU	B	542	-10.250	5.050	20.468	1.00	30.84
ATOM	3768	CG	GLU	B	542	-11.166	6.245	20.347	1.00	37.20
ATOM	3769	CD	GLU	B	542	-11.138	7.105	21.597	1.00	39.98
ATOM	3770	OE1	GLU	B	542	-12.223	7.385	22.144	1.00	39.92
ATOM	3771	OE2	GLU	B	542	-10.028	7.494	22.034	1.00	38.96
ATOM	3772	C	GLU	B	542	-8.826	4.010	18.724	1.00	27.90
ATOM	3773	O	GLU	B	542	-8.530	4.492	17.634	1.00	29.32
ATOM	3774	N	MET	B	543	-7.945	3.388	19.499	1.00	26.41
ATOM	3775	CA	MET	B	543	-6.552	3.237	19.107	1.00	23.53
ATOM	3776	CB	MET	B	543	-5.749	2.591	20.247	1.00	24.60
ATOM	3777	CG	MET	B	543	-5.812	3.338	21.579	1.00	26.46
ATOM	3778	SD	MET	B	543	-5.373	5.084	21.467	1.00	29.45
ATOM	3779	CE	MET	B	543	-3.585	4.971	21.349	1.00	25.43

ATOM	3780	C	MET	B	543	-6.403	2.407	17.832	1.00	25.80
ATOM	3781	O	MET	B	543	-5.535	2.686	17.004	1.00	23.59
ATOM	3782	N	LEU	B	544	-7.254	1.394	17.673	1.00	27.74
ATOM	3783	CA	LEU	B	544	-7.202	0.522	16.499	1.00	26.32
ATOM	3784	CB	LEU	B	544	-8.069	-0.721	16.719	1.00	26.75
ATOM	3785	CG	LEU	B	544	-8.274	-1.632	15.502	1.00	28.12
ATOM	3786	CD1	LEU	B	544	-6.956	-2.294	15.136	1.00	26.36
ATOM	3787	CD2	LEU	B	544	-9.330	-2.680	15.803	1.00	27.00
ATOM	3788	C	LEU	B	544	-7.672	1.252	15.250	1.00	26.97
ATOM	3789	O	LEU	B	544	-7.036	1.181	14.195	1.00	24.25
ATOM	3790	N	ASP	B	545	-8.787	1.961	15.372	1.00	30.37
ATOM	3791	CA	ASP	B	545	-9.338	2.702	14.244	1.00	32.34
ATOM	3792	CB	ASP	B	545	-10.668	3.346	14.637	1.00	36.61
ATOM	3793	CG	ASP	B	545	-11.818	2.370	14.565	1.00	42.73
ATOM	3794	OD1	ASP	B	545	-12.858	2.624	15.211	1.00	47.39
ATOM	3795	OD2	ASP	B	545	-11.676	1.342	13.863	1.00	46.96
ATOM	3796	C	ASP	B	545	-8.382	3.762	13.711	1.00	31.27
ATOM	3797	O	ASP	B	545	-8.443	4.120	12.532	1.00	30.53
ATOM	3798	N	ALA	B	546	-7.506	4.272	14.572	1.00	29.02
ATOM	3799	CA	ALA	B	546	-6.543	5.280	14.141	1.00	31.21
ATOM	3800	CB	ALA	B	546	-5.646	5.693	15.306	1.00	30.98
ATOM	3801	C	ALA	B	546	-5.697	4.731	12.996	1.00	32.14
ATOM	3802	O	ALA	B	546	-5.189	5.490	12.170	1.00	33.78
ATOM	3803	N	HIS	B	547	-5.555	3.410	12.943	1.00	32.27
ATOM	3804	CA	HIS	B	547	-4.773	2.767	11.892	1.00	37.73
ATOM	3805	CB	HIS	B	547	-3.991	1.576	12.457	1.00	35.83
ATOM	3806	CG	HIS	B	547	-2.796	1.968	13.269	1.00	34.54
ATOM	3807	CD2	HIS	B	547	-2.698	2.553	14.486	1.00	30.23
ATOM	3808	ND1	HIS	B	547	-1.502	1.755	12.840	1.00	34.23
ATOM	3809	CE1	HIS	B	547	-0.659	2.193	13.760	1.00	36.72
ATOM	3810	NE2	HIS	B	547	-1.360	2.681	14.768	1.00	31.48
ATOM	3811	C	HIS	B	547	-5.649	2.286	10.735	1.00	43.69
ATOM	3812	O	HIS	B	547	-5.178	2.152	9.606	1.00	46.04
ATOM	3813	N	ARG	B	548	-6.919	2.020	11.019	1.00	48.35
ATOM	3814	CA	ARG	B	548	-7.843	1.551	9.993	1.00	54.74
ATOM	3815	CB	ARG	B	548	-8.522	0.267	10.452	1.00	54.66
ATOM	3816	C	ARG	B	548	-8.886	2.619	9.681	1.00	59.94
ATOM	3817	O	ARG	B	548	-8.580	3.812	9.672	1.00	62.81
ATOM	3818	N	LEU	B	549	-10.116	2.186	9.422	1.00	64.81
ATOM	3819	CA	LEU	B	549	-11.204	3.109	9.112	1.00	67.59
ATOM	3820	CB	LEU	B	549	-12.478	2.327	8.799	1.00	68.06
ATOM	3821	C	LEU	B	549	-11.449	4.069	10.275	1.00	69.12
ATOM	3822	O	LEU	B	549	-11.451	5.297	10.036	1.00	68.96
ATOM	3823	OXT	LEU	B	549	-11.634	3.579	11.412	1.00	70.70
HETATM	3824	CP9	DES	B	600	-4.547	-6.077	22.000	1.00	18.55
HETATM	3825	CP8	DES	B	600	-3.163	-6.365	21.467	1.00	17.72
HETATM	3826	CP7	DES	B	600	-2.897	-7.853	21.381	1.00	21.17
HETATM	3827	CP6	DES	B	600	-3.719	-8.551	20.374	1.00	22.05

HETATM	3828	CP1	DES	B	600	-3.405	-8.481	18.998	1.00	21.32
HETATM	3829	CP2	DES	B	600	-4.239	-9.095	18.063	1.00	21.61
HETATM	3830	CP3	DES	B	600	-5.388	-9.771	18.509	1.00	24.89
HETATM	3831	OP3	DES	B	600	-6.244	-10.339	17.600	1.00	24.94
HETATM	3832	CP4	DES	B	600	-5.718	-9.858	19.860	1.00	24.08
HETATM	3833	CP5	DES	B	600	-4.877	-9.240	20.791	1.00	24.67
HETATM	3834	C7	DES	B	600	-1.998	-8.460	22.190	1.00	16.67
HETATM	3835	C6	DES	B	600	-1.330	-7.834	23.325	1.00	15.39
HETATM	3836	C5	DES	B	600	-2.054	-7.642	24.522	1.00	17.62
HETATM	3837	C4	DES	B	600	-1.433	-7.072	25.634	1.00	16.16
HETATM	3838	C3	DES	B	600	-0.077	-6.685	25.542	1.00	20.04
HETATM	3839	O3	DES	B	600	0.509	-6.113	26.655	1.00	15.55
HETATM	3840	C2	DES	B	600	0.669	-6.866	24.353	1.00	18.94
HETATM	3841	C1	DES	B	600	0.035	-7.440	23.241	1.00	15.20
HETATM	3842	C8	DES	B	600	-1.642	-9.903	21.942	1.00	17.61
HETATM	3843	C9	DES	B	600	-0.440	-10.009	20.998	1.00	11.63
HETATM	3844	C1	CBM	B	417	-4.997	-22.994	25.273	1.00	55.80
HETATM	3845	O4	CBM	B	417	-4.789	-24.187	25.003	1.00	55.56
HETATM	3846	O3	CBM	B	417	-4.798	-22.559	26.552	1.00	56.04
HETATM	3847	C2	CBM	B	417	-5.468	-21.960	24.264	1.00	57.04
HETATM	3848	C1	CBM	B	530	-15.278	-5.124	10.243	1.00	87.39
HETATM	3849	O4	CBM	B	530	-15.852	-5.086	9.064	1.00	87.68
HETATM	3850	O3	CBM	B	530	-15.832	-4.291	11.201	1.00	86.22
HETATM	3851	C2	CBM	B	530	-14.207	-5.886	10.628	1.00	87.65
ATOM	3852	CB	HIS	C	687	9.818	-20.030	-2.211	1.00	63.34
ATOM	3853	C	HIS	C	687	10.133	-20.267	-4.689	1.00	63.49
ATOM	3854	O	HIS	C	687	11.204	-20.840	-4.472	1.00	63.87
ATOM	3855	N	HIS	C	687	7.944	-19.563	-3.758	1.00	65.42
ATOM	3856	CA	HIS	C	687	9.424	-19.484	-3.586	1.00	64.86
ATOM	3857	N	LYS	C	688	9.533	-20.281	-5.875	1.00	62.00
ATOM	3858	CA	LYS	C	688	10.101	-20.999	-7.009	1.00	60.81
ATOM	3859	CB	LYS	C	688	8.980	-21.540	-7.901	1.00	61.76
ATOM	3860	C	LYS	C	688	11.050	-20.127	-7.827	1.00	57.47
ATOM	3861	O	LYS	C	688	12.253	-20.379	-7.858	1.00	57.64
ATOM	3862	N	ILE	C	689	10.511	-19.103	-8.482	1.00	55.74
ATOM	3863	CA	ILE	C	689	11.326	-18.212	-9.306	1.00	53.09
ATOM	3864	CB	ILE	C	689	10.496	-17.057	-9.889	1.00	53.83
ATOM	3865	CG2	ILE	C	689	11.334	-16.286	-10.902	1.00	54.55
ATOM	3866	CG1	ILE	C	689	9.229	-17.603	-10.551	1.00	52.90
ATOM	3867	CD1	ILE	C	689	8.406	-16.550	-11.258	1.00	50.45
ATOM	3868	C	ILE	C	689	12.513	-17.611	-8.560	1.00	50.82
ATOM	3869	O	ILE	C	689	13.616	-17.550	-9.097	1.00	51.28
ATOM	3870	N	LEU	C	690	12.288	-17.162	-7.329	1.00	48.01
ATOM	3871	CA	LEU	C	690	13.362	-16.570	-6.534	1.00	47.33
ATOM	3872	CB	LEU	C	690	12.812	-16.058	-5.199	1.00	42.51
ATOM	3873	CG	LEU	C	690	13.835	-15.501	-4.206	1.00	40.67
ATOM	3874	CD1	LEU	C	690	14.575	-14.324	-4.831	1.00	39.95
ATOM	3875	CD2	LEU	C	690	13.128	-15.078	-2.926	1.00	38.77

ATOM	3876	C	LEU	C	690	14.445	-17.615	-6.282	1.00	48.87
ATOM	3877	O	LEU	C	690	15.643	-17.340	-6.393	1.00	46.71
ATOM	3878	N	HIS	C	691	14.001	-18.818	-5.939	1.00	51.36
ATOM	3879	CA	HIS	C	691	14.886	-19.946	-5.675	1.00	53.35
ATOM	3880	CB	HIS	C	691	14.042	-21.203	-5.460	1.00	58.64
ATOM	3881	CG	HIS	C	691	14.655	-22.195	-4.526	1.00	62.94
ATOM	3882	CD2	HIS	C	691	15.503	-23.227	-4.751	1.00	64.95
ATOM	3883	ND1	HIS	C	691	14.392	-22.202	-3.173	1.00	65.49
ATOM	3884	CE1	HIS	C	691	15.053	-23.195	-2.605	1.00	68.18
ATOM	3885	NE2	HIS	C	691	15.733	-23.833	-3.540	1.00	68.77
ATOM	3886	C	HIS	C	691	15.824	-20.162	-6.861	1.00	52.19
ATOM	3887	O	HIS	C	691	17.048	-20.153	-6.717	1.00	47.53
ATOM	3888	N	ARG	C	692	15.222	-20.350	-8.032	1.00	52.37
ATOM	3889	CA	ARG	C	692	15.949	-20.586	-9.271	1.00	52.90
ATOM	3890	CB	ARG	C	692	14.955	-20.832	-10.410	1.00	54.04
ATOM	3891	CG	ARG	C	692	15.575	-20.826	-11.797	1.00	57.52
ATOM	3892	CD	ARG	C	692	14.528	-21.048	-12.874	1.00	58.25
ATOM	3893	NE	ARG	C	692	14.375	-19.878	-13.732	1.00	61.43
ATOM	3894	CZ	ARG	C	692	13.218	-19.260	-13.951	1.00	64.32
ATOM	3895	NH1	ARG	C	692	12.108	-19.706	-13.378	1.00	63.22
ATOM	3896	NH2	ARG	C	692	13.171	-18.197	-14.746	1.00	65.93
ATOM	3897	C	ARG	C	692	16.873	-19.434	-9.639	1.00	53.09
ATOM	3898	O	ARG	C	692	18.047	-19.644	-9.956	1.00	53.06
ATOM	3899	N	LEU	C	693	16.338	-18.217	-9.607	1.00	50.73
ATOM	3900	CA	LEU	C	693	17.125	-17.039	-9.945	1.00	49.53
ATOM	3901	CB	LEU	C	693	16.249	-15.784	-9.881	1.00	49.56
ATOM	3902	CG	LEU	C	693	15.781	-15.245	-11.239	1.00	49.78
ATOM	3903	CD1	LEU	C	693	15.219	-16.389	-12.079	1.00	50.30
ATOM	3904	CD2	LEU	C	693	14.728	-14.170	-11.037	1.00	48.79
ATOM	3905	C	LEU	C	693	18.318	-16.904	-9.006	1.00	48.38
ATOM	3906	O	LEU	C	693	19.382	-16.426	-9.402	1.00	46.35
ATOM	3907	N	LEU	C	694	18.135	-17.329	-7.761	1.00	46.74
ATOM	3908	CA	LEU	C	694	19.204	-17.272	-6.775	1.00	49.41
ATOM	3909	CB	LEU	C	694	18.634	-17.415	-5.362	1.00	45.20
ATOM	3910	CG	LEU	C	694	18.222	-16.128	-4.643	1.00	40.19
ATOM	3911	CD1	LEU	C	694	17.456	-16.474	-3.371	1.00	41.65
ATOM	3912	CD2	LEU	C	694	19.453	-15.307	-4.317	1.00	35.91
ATOM	3913	C	LEU	C	694	20.172	-18.417	-7.058	1.00	54.15
ATOM	3914	O	LEU	C	694	21.370	-18.320	-6.776	1.00	53.55
ATOM	3915	N	GLN	C	695	19.634	-19.498	-7.619	1.00	57.44
ATOM	3916	CA	GLN	C	695	20.416	-20.685	-7.959	1.00	62.46
ATOM	3917	CB	GLN	C	695	19.477	-21.853	-8.304	1.00	61.95
ATOM	3918	CG	GLN	C	695	19.548	-23.010	-7.311	1.00	61.49
ATOM	3919	CD	GLN	C	695	18.454	-24.053	-7.490	1.00	62.78
ATOM	3920	OE1	GLN	C	695	18.262	-24.928	-6.653	1.00	63.33
ATOM	3921	NE2	GLN	C	695	17.720	-23.969	-8.608	1.00	60.37
ATOM	3922	C	GLN	C	695	21.330	-20.414	-9.149	1.00	65.13
ATOM	3923	O	GLN	C	695	22.517	-20.740	-9.116	1.00	65.87

ATOM	3924	N	ASP	C	696	20.761	-19.824	-10.197	1.00	67.67
ATOM	3925	CA	ASP	C	696	21.492	-19.500	-11.420	1.00	70.66
ATOM	3926	CB	ASP	C	696	20.801	-18.348	-12.151	1.00	71.06
ATOM	3927	CG	ASP	C	696	20.127	-18.792	-13.430	1.00	71.70
ATOM	3928	OD1	ASP	C	696	20.637	-18.455	-14.521	1.00	72.47
ATOM	3929	OD2	ASP	C	696	19.086	-19.478	-13.342	1.00	71.41
ATOM	3930	C	ASP	C	696	22.951	-19.132	-11.169	1.00	72.41
ATOM	3931	O	ASP	C	696	23.245	-18.115	-10.541	1.00	72.56
ATOM	3932	N	SER	C	697	23.859	-19.967	-11.668	1.00	74.67
ATOM	3933	CA	SER	C	697	25.291	-19.741	-11.507	1.00	76.45
ATOM	3934	CB	SER	C	697	26.019	-21.076	-11.377	1.00	76.00
ATOM	3935	C	SER	C	697	25.841	-18.960	-12.696	1.00	78.44
ATOM	3936	O	SER	C	697	26.286	-17.809	-12.489	1.00	79.20
ATOM	3937	OXT	SER	C	697	25.818	-19.510	-13.820	1.00	80.07
ATOM	3938	CB	LYS	D	686	-14.070	13.661	16.843	1.00	50.28
ATOM	3939	C	LYS	D	686	-13.682	14.418	19.199	1.00	51.59
ATOM	3940	O	LYS	D	686	-12.629	14.738	19.759	1.00	50.42
ATOM	3941	N	LYS	D	686	-12.910	15.796	17.283	1.00	50.43
ATOM	3942	CA	LYS	D	686	-13.976	14.872	17.769	1.00	50.62
ATOM	3943	N	HIS	D	687	-14.617	13.676	19.787	1.00	49.91
ATOM	3944	CA	HIS	D	687	-14.447	13.176	21.144	1.00	51.28
ATOM	3945	CB	HIS	D	687	-15.806	12.984	21.828	1.00	54.12
ATOM	3946	CG	HIS	D	687	-15.713	12.336	23.177	1.00	60.06
ATOM	3947	CD2	HIS	D	687	-15.418	11.064	23.539	1.00	61.05
ATOM	3948	ND1	HIS	D	687	-15.911	13.030	24.352	1.00	62.39
ATOM	3949	CE1	HIS	D	687	-15.741	12.215	25.378	1.00	62.76
ATOM	3950	NE2	HIS	D	687	-15.441	11.016	24.912	1.00	63.46
ATOM	3951	C	HIS	D	687	-13.691	11.849	21.163	1.00	49.55
ATOM	3952	O	HIS	D	687	-14.099	10.878	20.524	1.00	50.84
ATOM	3953	N	LYS	D	688	-12.593	11.816	21.909	1.00	44.00
ATOM	3954	CA	LYS	D	688	-11.784	10.611	22.038	1.00	40.31
ATOM	3955	CB	LYS	D	688	-10.446	10.773	21.299	1.00	41.42
ATOM	3956	CG	LYS	D	688	-10.513	10.595	19.780	1.00	42.76
ATOM	3957	CD	LYS	D	688	-9.123	10.716	19.152	1.00	38.66
ATOM	3958	CE	LYS	D	688	-9.162	10.529	17.640	1.00	38.28
ATOM	3959	NZ	LYS	D	688	-7.894	10.970	16.986	1.00	31.58
ATOM	3960	C	LYS	D	688	-11.506	10.378	23.517	1.00	36.70
ATOM	3961	O	LYS	D	688	-11.271	11.326	24.266	1.00	33.38
ATOM	3962	N	ILE	D	689	-11.549	9.122	23.942	1.00	33.06
ATOM	3963	CA	ILE	D	689	-11.255	8.806	25.328	1.00	28.70
ATOM	3964	CB	ILE	D	689	-11.438	7.301	25.607	1.00	30.88
ATOM	3965	CG2	ILE	D	689	-10.725	6.912	26.899	1.00	31.45
ATOM	3966	CG1	ILE	D	689	-12.927	6.971	25.721	1.00	32.57
ATOM	3967	CD1	ILE	D	689	-13.308	5.679	25.031	1.00	29.79
ATOM	3968	C	ILE	D	689	-9.790	9.193	25.541	1.00	27.64
ATOM	3969	O	ILE	D	689	-9.405	9.649	26.611	1.00	25.54
ATOM	3970	N	LEU	D	690	-8.985	9.021	24.496	1.00	24.25
ATOM	3971	CA	LEU	D	690	-7.563	9.348	24.549	1.00	26.63

	ATOM	3972	CB	LEU	D	690	-6.903	9.021	23.200	1.00	22.83
	ATOM	3973	CG	LEU	D	690	-5.433	9.387	22.992	1.00	25.47
	ATOM	3974	CD1	LEU	D	690	-4.595	8.772	24.108	1.00	24.03
	ATOM	3975	CD2	LEU	D	690	-4.956	8.898	21.616	1.00	20.87
	ATOM	3976	C	LEU	D	690	-7.344	10.823	24.902	1.00	26.64
	ATOM	3977	O	LEU	D	690	-6.408	11.165	25.625	1.00	28.34
	ATOM	3978	N	HIS	D	691	-8.206	11.694	24.383	1.00	27.77
	ATOM	3979	CA	HIS	D	691	-8.107	13.125	24.665	1.00	29.16
	ATOM	3980	CB	HIS	D	691	-9.156	13.907	23.861	1.00	30.89
	ATOM	3981	CG	HIS	D	691	-8.903	13.935	22.386	1.00	37.09
	ATOM	3982	CD2	HIS	D	691	-7.750	14.000	21.679	1.00	41.39
	ATOM	3983	ND1	HIS	D	691	-9.920	13.906	21.458	1.00	41.65
	ATOM	3984	CE1	HIS	D	691	-9.407	13.953	20.242	1.00	44.64
	ATOM	3985	NE2	HIS	D	691	-8.091	14.010	20.347	1.00	41.94
	ATOM	3986	C	HIS	D	691	-8.338	13.373	26.159	1.00	26.65
	ATOM	3987	O	HIS	D	691	-7.602	14.120	26.802	1.00	24.50
	ATOM	3988	N	ARG	D	692	-9.371	12.742	26.703	1.00	25.70
	ATOM	3989	CA	ARG	D	692	-9.691	12.912	28.114	1.00	29.11
	ATOM	3990	CB	ARG	D	692	-10.959	12.134	28.472	1.00	30.84
	ATOM	3991	CG	ARG	D	692	-11.255	12.129	29.963	1.00	41.63
	ATOM	3992	CD	ARG	D	692	-12.502	11.327	30.290	1.00	48.83
	ATOM	3993	NE	ARG	D	692	-13.618	12.198	30.647	1.00	54.50
	ATOM	3994	CZ	ARG	D	692	-14.498	12.677	29.774	1.00	59.37
	ATOM	3995	NH1	ARG	D	692	-14.392	12.371	28.486	1.00	60.97
	ATOM	3996	NH2	ARG	D	692	-15.483	13.464	30.188	1.00	59.07
	ATOM	3997	C	ARG	D	692	-8.548	12.451	29.011	1.00	28.30
	ATOM	3998	O	ARG	D	692	-8.139	13.167	29.929	1.00	26.50
	ATOM	3999	N	LEU	D	693	-8.030	11.259	28.737	1.00	24.87
	ATOM	4000	CA	LEU	D	693	-6.943	10.705	29.536	1.00	27.17
	ATOM	4001	CB	LEU	D	693	-6.674	9.254	29.116	1.00	28.45
	ATOM	4002	CG	LEU	D	693	-7.844	8.300	29.391	1.00	30.40
	ATOM	4003	CD1	LEU	D	693	-7.575	6.932	28.778	1.00	34.79
	ATOM	4004	CD2	LEU	D	693	-8.043	8.171	30.894	1.00	32.02
	ATOM	4005	C	LEU	D	693	-5.670	11.539	29.440	1.00	25.96
	ATOM	4006	O	LEU	D	693	-4.948	11.700	30.428	1.00	27.01
	ATOM	4007	N	LEU	D	694	-5.395	12.080	28.257	1.00	25.33
	ATOM	4008	CA	LEU	D	694	-4.207	12.906	28.062	1.00	27.22
	ATOM	4009	CB	LEU	D	694	-3.948	13.126	26.572	1.00	24.61
	ATOM	4010	CG	LEU	D	694	-3.118	12.080	25.825	1.00	22.20
	ATOM	4011	CD1	LEU	D	694	-3.230	12.332	24.324	1.00	21.13
	ATOM	4012	CD2	LEU	D	694	-1.666	12.148	26.275	1.00	21.34
	ATOM	4013	C	LEU	D	694	-4.336	14.270	28.742	1.00	32.40
	ATOM	4014	O	LEU	D	694	-3.339	14.889	29.102	1.00	31.55
	ATOM	4015	N	GLN	D	695	-5.570	14.733	28.915	1.00	36.93
	ATOM	4016	CA	GLN	D	695	-5.820	16.032	29.528	1.00	43.18
	ATOM	4017	CB	GLN	D	695	-7.022	16.694	28.862	1.00	40.48
	ATOM	4018	CG	GLN	D	695	-6.772	17.071	27.422	1.00	37.99
	ATOM	4019	CD	GLN	D	695	-7.943	17.764	26.795	1.00	35.86

ATOM	4020	OE1	GLN	D	695	-7.863	18.895	26.342	1.00	38.84
ATOM	4021	NE2	GLN	D	695	-9.082	17.060	26.757	1.00	31.62
ATOM	4022	C	GLN	D	695	-6.049	16.009	31.034	1.00	48.74
ATOM	4023	O	GLN	D	695	-6.119	17.065	31.660	1.00	51.25
ATOM	4024	N	ASP	D	696	-6.175	14.818	31.611	1.00	54.01
ATOM	4025	CA	ASP	D	696	-6.398	14.702	33.047	1.00	62.23
ATOM	4026	CB	ASP	D	696	-6.217	13.238	33.485	1.00	63.97
ATOM	4027	CG	ASP	D	696	-7.527	12.467	33.475	1.00	67.72
ATOM	4028	OD1	ASP	D	696	-8.528	12.996	32.941	1.00	68.11
ATOM	4029	OD2	ASP	D	696	-7.552	11.333	34.003	1.00	68.95
ATOM	4030	C	ASP	D	696	-5.456	15.622	33.840	1.00	65.60
ATOM	4031	O	ASP	D	696	-4.312	15.189	34.134	1.00	68.33
ATOM	4032	OXT	ASP	D	696	-5.874	16.755	34.140	1.00	69.20
HETATM	4033	O	HOH		1	16.153	-0.605	-4.425	1.00	17.11
HETATM	4034	O	HOH		2	16.570	-5.304	-16.560	1.00	21.44
HETATM	4035	O	HOH		3	18.526	0.742	-4.495	1.00	23.43
HETATM	4036	O	HOH		4	13.647	-2.187	8.588	1.00	25.82
HETATM	4037	O	HOH		5	9.778	-5.825	2.509	1.00	20.58
HETATM	4038	O	HOH		6	17.072	-3.605	-8.015	1.00	18.38
HETATM	4039	O	HOH		7	24.920	-1.689	-2.780	1.00	25.74
HETATM	4040	O	HOH		8	7.321	-5.649	5.061	1.00	24.11
HETATM	4041	O	HOH		9	25.976	-3.535	15.158	1.00	26.78
HETATM	4042	O	HOH		10	15.088	-7.006	-15.192	1.00	19.64
HETATM	4043	O	HOH		11	14.070	0.925	-5.953	1.00	20.55
HETATM	4044	O	HOH		12	18.008	3.407	-6.654	1.00	32.30
HETATM	4045	O	HOH		13	31.949	-8.393	13.487	1.00	30.64
HETATM	4046	O	HOH		14	19.625	-2.804	-4.279	1.00	24.45
HETATM	4047	O	HOH		15	11.741	1.079	-21.140	1.00	25.87
HETATM	4048	O	HOH		16	25.067	13.951	14.153	1.00	31.07
HETATM	4049	O	HOH		17	15.501	1.323	-10.393	1.00	21.01
HETATM	4050	O	HOH		18	13.880	3.349	-11.482	1.00	24.28
HETATM	4051	O	HOH		19	17.591	0.979	-8.828	1.00	35.26
HETATM	4052	O	HOH		20	23.682	-2.041	-0.314	1.00	37.90
HETATM	4053	O	HOH		21	15.754	9.496	11.841	1.00	39.44
HETATM	4054	O	HOH		22	-4.943	7.574	-3.066	1.00	37.67
HETATM	4055	O	HOH		23	6.877	0.354	-15.982	1.00	36.92
HETATM	4056	O	HOH		24	15.806	-4.002	8.671	1.00	30.38
HETATM	4057	O	HOH		25	17.185	-3.158	-5.321	1.00	28.89
HETATM	4058	O	HOH		26	17.572	9.249	17.009	1.00	30.15
HETATM	4059	O	HOH		27	24.096	-2.929	11.604	1.00	31.37
HETATM	4060	O	HOH		28	22.324	-5.871	-11.980	1.00	32.74
HETATM	4061	O	HOH		29	27.547	-12.361	-0.801	1.00	36.61
HETATM	4062	O	HOH		30	11.173	13.442	-2.719	1.00	35.41
HETATM	4063	O	HOH		31	15.438	-9.527	5.483	1.00	29.88
HETATM	4064	O	HOH		32	9.946	-6.564	5.983	1.00	35.05
HETATM	4065	O	HOH		33	7.599	11.680	-15.261	1.00	38.68
HETATM	4066	O	HOH		34	20.112	10.503	-5.109	1.00	42.66
HETATM	4067	O	HOH		35	15.972	10.343	14.897	1.00	41.73

	HETATM 4068	O	HOH	36	22.401	-5.914	-9.527	1.00	28.08
	HETATM 4069	O	HOH	37	16.128	-0.899	-8.109	1.00	33.13
	HETATM 4070	O	HOH	38	3.581	15.655	-3.706	1.00	41.37
	HETATM 4071	O	HOH	39	31.900	13.545	21.339	1.00	37.79
5	HETATM 4072	O	HOH	40	20.058	-7.530	14.119	1.00	47.51
	HETATM 4073	O	HOH	41	34.634	6.668	15.632	1.00	29.24
	HETATM 4074	O	HOH	42	17.968	10.511	-9.085	1.00	44.60
	HETATM 4075	O	HOH	43	23.258	-17.325	-4.088	1.00	44.10
	HETATM 4076	O	HOH	44	4.034	-1.472	27.521	1.00	15.22
10	HETATM 4077	O	HOH	45	-5.943	-0.018	36.088	1.00	21.11
	HETATM 4078	O	HOH	46	6.084	-1.509	29.478	1.00	19.51
	HETATM 4079	O	HOH	47	9.762	1.061	15.621	1.00	27.74
	HETATM 4080	O	HOH	48	1.804	0.717	17.260	1.00	20.97
	HETATM 4081	O	HOH	49	0.929	0.421	30.281	1.00	19.64
15	HETATM 4082	O	HOH	50	9.627	4.271	31.231	1.00	19.02
	HETATM 4083	O	HOH	51	2.121	-0.261	13.654	1.00	26.09
	HETATM 4084	O	HOH	52	20.060	10.275	17.711	1.00	25.49
	HETATM 4085	O	HOH	53	-6.786	0.736	33.483	1.00	22.34
	HETATM 4086	O	HOH	54	2.751	-4.136	27.760	1.00	19.93
20	HETATM 4087	O	HOH	55	5.994	-4.079	31.292	1.00	32.27
	HETATM 4088	O	HOH	56	19.416	16.921	21.645	1.00	25.54
	HETATM 4089	O	HOH	57	4.833	2.325	29.006	1.00	19.00
	HETATM 4090	O	HOH	58	-7.638	-8.931	37.809	1.00	24.79
	HETATM 4091	O	HOH	59	28.442	-4.673	21.875	1.00	24.32
25	HETATM 4092	O	HOH	60	1.094	-4.893	32.100	1.00	24.27
	HETATM 4093	O	HOH	61	0.905	-7.306	32.783	1.00	21.33
	HETATM 4094	O	HOH	62	3.396	-2.971	32.306	1.00	26.13
	HETATM 4095	O	HOH	63	10.363	4.576	28.391	1.00	33.43
	HETATM 4096	O	HOH	64	19.551	-6.473	16.597	1.00	35.38
30	HETATM 4097	O	HOH	65	-2.888	-19.627	15.665	1.00	27.99
	HETATM 4098	O	HOH	66	-7.275	-9.745	31.077	1.00	27.00
	HETATM 4099	O	HOH	67	10.189	3.580	16.510	1.00	24.19
	HETATM 4100	O	HOH	68	2.741	0.716	28.382	1.00	16.48
	HETATM 4101	O	HOH	69	23.522	-4.323	13.943	1.00	27.48
35	HETATM 4102	O	HOH	70	17.133	8.133	19.686	1.00	32.24
	HETATM 4103	O	HOH	71	-0.295	4.535	35.884	1.00	33.42
	HETATM 4104	O	HOH	72	9.519	10.828	34.842	1.00	29.38
	HETATM 4105	O	HOH	73	6.291	14.878	29.070	1.00	28.21
	HETATM 4106	O	HOH	74	-1.721	6.480	13.381	1.00	49.91
40	HETATM 4107	O	HOH	75	10.091	-15.427	26.194	1.00	24.17
	HETATM 4108	O	HOH	76	5.029	7.461	17.718	1.00	18.91
	HETATM 4109	O	HOH	77	3.758	2.086	14.306	1.00	28.28
	HETATM 4110	O	HOH	78	-1.390	-18.739	33.183	1.00	41.11
	HETATM 4111	O	HOH	79	12.703	-8.687	32.119	1.00	36.21
45	HETATM 4112	O	HOH	80	22.270	-6.451	14.844	1.00	33.21
	HETATM 4113	O	HOH	81	1.458	4.605	34.026	1.00	23.59
	HETATM 4114	O	HOH	82	1.759	-2.158	30.374	1.00	28.78
	HETATM 4115	O	HOH	83	6.153	-21.372	23.188	1.00	31.14

	HETATM 4116	O	HOH	84	36.525	0.463	20.792	1.00	45.26
	HETATM 4117	O	HOH	85	13.832	9.696	13.792	1.00	33.12
	HETATM 4118	O	HOH	86	31.166	6.635	24.924	1.00	35.19
	HETATM 4119	O	HOH	87	8.844	-10.389	34.180	1.00	48.80
	HETATM 4120	O	HOH	88	9.581	-6.956	34.136	1.00	42.95
	HETATM 4121	O	HOH	89	-1.563	15.887	27.596	1.00	39.35
	HETATM 4122	O	HOH	90	-5.286	10.345	32.757	1.00	35.20
	HETATM 4123	O	HOH	91	15.035	0.607	13.339	1.00	29.53
	HETATM 4124	O	HOH	92	-10.984	-1.500	30.272	1.00	29.84
	HETATM 4125	O	HOH	93	-7.239	-0.271	-1.207	1.00	48.98
	HETATM 4126	O	HOH	94	18.022	-4.902	34.286	1.00	35.28
	HETATM 4127	O	HOH	95	29.347	-6.319	19.920	1.00	37.20
	HETATM 4128	O	HOH	96	-14.309	-19.369	20.945	1.00	30.23
	HETATM 4129	O	HOH	97	31.496	4.614	18.716	1.00	38.79
	HETATM 4130	O	HOH	98	26.567	9.759	25.629	1.00	29.72
	HETATM 4131	O	HOH	99	2.848	14.531	1.134	1.00	38.08
	HETATM 4132	O	HOH	100	-9.373	5.699	-7.953	1.00	53.23
	HETATM 4133	O	HOH	101	-10.137	-0.553	-6.742	1.00	47.72
	HETATM 4134	O	HOH	102	10.558	-10.363	15.403	1.00	40.97
	HETATM 4135	O	HOH	103	21.079	17.166	18.929	1.00	32.40
	HETATM 4136	O	HOH	104	25.810	-5.921	22.506	1.00	37.69
	HETATM 4137	O	HOH	105	22.493	-1.311	34.465	1.00	49.94
	HETATM 4138	O	HOH	106	19.317	10.977	38.703	1.00	40.60
	HETATM 4139	O	HOH	107	4.479	13.951	3.045	1.00	45.33
	HETATM 4140	O	HOH	108	20.418	19.353	34.044	1.00	42.18
	HETATM 4141	O	HOH	109	-3.065	8.936	14.062	1.00	38.41
	HETATM 4142	O	HOH	110	26.856	-4.674	-10.940	1.00	55.67
	HETATM 4143	O	HOH	111	2.032	-6.387	5.614	1.00	42.23
	HETATM 4144	O	HOH	112	0.601	0.228	-17.268	1.00	40.57
	HETATM 4145	O	HOH	113	4.903	13.488	-14.050	1.00	47.72
	HETATM 4146	O	HOH	114	3.986	16.140	-0.960	1.00	40.66
	HETATM 4147	O	HOH	115	12.968	-19.561	2.741	1.00	40.76
	HETATM 4148	O	HOH	116	7.170	15.583	2.599	1.00	43.69
	HETATM 4149	O	HOH	117	-1.966	10.606	3.572	1.00	52.63
	HETATM 4150	O	HOH	118	29.030	10.644	6.707	1.00	42.54
	HETATM 4151	O	HOH	119	0.468	4.354	8.374	1.00	38.69
	HETATM 4152	O	HOH	120	29.086	17.119	19.272	1.00	45.51
	HETATM 4153	O	HOH	121	24.614	17.609	20.174	1.00	53.55
	HETATM 4154	O	HOH	122	-15.318	0.362	26.686	1.00	36.77
	HETATM 4155	O	HOH	123	-3.857	-24.786	28.325	1.00	39.64
	HETATM 4156	O	HOH	124	21.728	22.178	31.983	1.00	43.73
	HETATM 4157	O	HOH	125	31.650	-7.370	21.642	1.00	40.53
	HETATM 4158	O	HOH	126	25.421	10.436	21.161	1.00	32.31
	HETATM 4159	O	HOH	127	10.317	-9.457	12.998	1.00	37.77
	HETATM 4160	O	HOH	128	22.723	14.887	15.427	1.00	47.90
	HETATM 4161	O	HOH	129	6.702	9.556	37.596	1.00	47.81
	HETATM 4162	O	HOH	130	27.987	13.557	7.167	1.00	41.15
	HETATM 4163	O	HOH	131	30.798	16.499	7.588	1.00	58.47

HETATM 4164	O	HOH	132	10.071	-0.571	-20.393	1.00	38.79
HETATM 4165	O	HOH	133	9.562	8.334	-21.392	1.00	36.80
HETATM 4166	O	HOH	134	6.712	6.058	8.822	1.00	37.43
HETATM 4167	O	HOH	135	5.927	8.454	10.594	1.00	42.34
HETATM 4168	O	HOH	136	4.472	6.306	10.973	1.00	37.35
HETATM 4169	O	HOH	137	6.792	7.721	7.051	1.00	47.23
HETATM 4170	O	HOH	138	24.513	11.582	33.724	1.00	45.55
HETATM 4171	O	HOH	139	-2.528	-20.361	12.354	1.00	52.13
HETATM 4172	O	HOH	140	-7.864	7.706	19.248	1.00	47.82
HETATM 4173	O	HOH	141	11.577	-16.962	24.398	1.00	39.43
HETATM 4174	O	HOH	142	18.087	12.263	-5.507	1.00	33.36
HETATM 4175	O	HOH	143	-6.816	-14.190	10.674	1.00	51.32
HETATM 4176	O	HOH	144	-7.377	-16.701	33.528	1.00	57.11
HETATM 4177	O	HOH	145	-5.379	-20.107	32.689	1.00	43.01
HETATM 4178	O	HOH	146	8.766	-7.947	-16.274	1.00	49.96
HETATM 4179	O	HOH	147	10.946	-7.937	-18.142	1.00	55.67
END								

Appendix 2

Atomic Coordinates for Human ERα Complexed With OHT

CRYST1	58.242	58.242	277.467	90.00	90.00	120.00	P	65	2	2 12
ORIGX1	1.000000	0.000000	0.000000	0.00000						
ORIGX2	0.000000	1.000000	0.000000	0.00000						
ORIGX3	0.000000	0.000000	1.000000	0.00000						
SCALE1	0.017170	0.009913	0.000000	0.00000						
SCALE2	0.000000	0.019826	0.000000	0.00000						
SCALE3	0.000000	0.000000	0.003604	0.00000						
ATOM	1	CB	LEU	306	6.638	11.502	3.989	1.00	61.20	
ATOM	2	C	LEU	306	7.381	10.684	6.231	1.00	61.47	
ATOM	3	O	LEU	306	6.407	11.020	6.905	1.00	62.09	
ATOM	4	N	LEU	306	6.369	9.128	4.588	1.00	62.32	
ATOM	5	CA	LEU	306	7.232	10.330	4.754	1.00	61.30	
ATOM	6	N	ALA	307	8.609	10.605	6.730	1.00	60.52	
ATOM	7	CA	ALA	307	8.891	10.912	8.125	1.00	58.77	
ATOM	8	CB	ALA	307	10.318	10.501	8.465	1.00	59.70	
ATOM	9	C	ALA	307	8.692	12.393	8.429	1.00	57.51	
ATOM	10	O	ALA	307	8.451	12.770	9.574	1.00	57.64	
ATOM	11	N	LEU	308	8.789	13.228	7.400	1.00	55.82	
ATOM	12	CA	LEU	308	8.638	14.668	7.573	1.00	56.62	
ATOM	13	CB	LEU	308	9.298	15.402	6.406	1.00	57.48	
ATOM	14	CG	LEU	308	10.637	14.822	5.948	1.00	59.17	
ATOM	15	CD1	LEU	308	10.474	14.189	4.569	1.00	60.38	
ATOM	16	CD2	LEU	308	11.694	15.920	5.933	1.00	58.46	
ATOM	17	C	LEU	308	7.190	15.130	7.710	1.00	56.51	
ATOM	18	O	LEU	308	6.935	16.307	7.961	1.00	55.58	
ATOM	19	N	SER	309	6.246	14.208	7.546	1.00	57.04	
ATOM	20	CA	SER	309	4.828	14.544	7.657	1.00	56.46	
ATOM	21	CB	SER	309	4.034	13.896	6.514	1.00	56.79	
ATOM	22	OG	SER	309	4.071	12.479	6.588	1.00	57.23	
ATOM	23	C	SER	309	4.261	14.095	9.003	1.00	56.13	
ATOM	24	O	SER	309	3.166	14.507	9.398	1.00	55.17	
ATOM	25	N	LEU	310	5.016	13.257	9.706	1.00	54.31	
ATOM	26	CA	LEU	310	4.591	12.749	11.004	1.00	53.55	
ATOM	27	CB	LEU	310	5.651	11.811	11.582	1.00	54.40	
ATOM	28	CG	LEU	310	5.586	10.333	11.189	1.00	56.49	
ATOM	29	CD1	LEU	310	5.530	10.200	9.676	1.00	57.06	
ATOM	30	CD2	LEU	310	6.809	9.610	11.739	1.00	57.28	
ATOM	31	C	LEU	310	4.330	13.865	12.003	1.00	53.18	
ATOM	32	O	LEU	310	4.993	14.905	11.984	1.00	53.17	
ATOM	33	N	THR	311	3.352	13.641	12.874	1.00	51.71	
ATOM	34	CA	THR	311	3.017	14.604	13.912	1.00	49.93	
ATOM	35	CB	THR	311	1.527	14.554	14.275	1.00	48.96	

	ATOM	36	OG1	THR	311	1.242	13.311	14.930	1.00	47.20
	ATOM	37	CG2	THR	311	0.666	14.688	13.027	1.00	50.99
	ATOM	38	C	THR	311	3.815	14.201	15.145	1.00	48.84
	ATOM	39	O	THR	311	4.371	13.103	15.197	1.00	46.66
	ATOM	40	N	ALA	312	3.857	15.078	16.141	1.00	48.76
	ATOM	41	CA	ALA	312	4.590	14.798	17.369	1.00	47.75
	ATOM	42	CB	ALA	312	4.359	15.910	18.378	1.00	47.06
	ATOM	43	C	ALA	312	4.171	13.460	17.964	1.00	47.41
	ATOM	44	O	ALA	312	5.009	12.609	18.262	1.00	45.52
	ATOM	45	N	ASP	313	2.868	13.275	18.143	1.00	47.58
	ATOM	46	CA	ASP	313	2.367	12.032	18.714	1.00	47.63
	ATOM	47	CB	ASP	313	0.848	12.100	18.879	1.00	51.96
	ATOM	48	CG	ASP	313	0.430	12.872	20.118	1.00	56.21
	ATOM	49	OD1	ASP	313	1.314	13.234	20.929	1.00	56.38
	ATOM	50	OD2	ASP	313	-0.785	13.117	20.282	1.00	59.15
	ATOM	51	C	ASP	313	2.745	10.846	17.835	1.00	43.93
	ATOM	52	O	ASP	313	2.959	9.741	18.330	1.00	44.77
	ATOM	53	N	GLN	314	2.826	11.081	16.531	1.00	44.52
	ATOM	54	CA	GLN	314	3.182	10.028	15.588	1.00	44.73
	ATOM	55	CB	GLN	314	2.849	10.464	14.156	1.00	45.05
	ATOM	56	CG	GLN	314	1.534	9.886	13.626	1.00	48.47
	ATOM	57	CD	GLN	314	0.982	10.646	12.428	1.00	50.37
	ATOM	58	OE1	GLN	314	1.649	11.515	11.856	1.00	49.38
	ATOM	59	NE2	GLN	314	-0.248	10.318	12.043	1.00	51.74
	ATOM	60	C	GLN	314	4.673	9.722	15.707	1.00	43.26
	ATOM	61	O	GLN	314	5.100	8.580	15.555	1.00	43.93
	ATOM	62	N	MET	315	5.459	10.757	15.980	1.00	42.29
	ATOM	63	CA	MET	315	6.901	10.606	16.130	1.00	41.26
	ATOM	64	CB	MET	315	7.565	11.985	16.224	1.00	42.43
	ATOM	65	CG	MET	315	9.082	11.939	16.356	1.00	42.34
	ATOM	66	SD	MET	315	9.906	11.190	14.925	1.00	46.22
	ATOM	67	CE	MET	315	9.547	12.408	13.680	1.00	37.32
	ATOM	68	C	MET	315	7.218	9.791	17.379	1.00	38.89
	ATOM	69	O	MET	315	8.002	8.841	17.335	1.00	40.02
	ATOM	70	N	VAL	316	6.599	10.165	18.491	1.00	37.65
	ATOM	71	CA	VAL	316	6.819	9.476	19.756	1.00	39.56
	ATOM	72	CB	VAL	316	6.023	10.136	20.897	1.00	39.22
	ATOM	73	CG1	VAL	316	6.245	9.373	22.192	1.00	44.43
	ATOM	74	CG2	VAL	316	6.446	11.583	21.059	1.00	41.04
	ATOM	75	C	VAL	316	6.404	8.012	19.664	1.00	40.04
	ATOM	76	O	VAL	316	7.141	7.117	20.077	1.00	37.86
	ATOM	77	N	SER	317	5.215	7.767	19.127	1.00	41.90
	ATOM	78	CA	SER	317	4.733	6.400	18.997	1.00	41.68
	ATOM	79	CB	SER	317	3.311	6.402	18.415	1.00	43.85
	ATOM	80	OG	SER	317	3.225	5.631	17.230	1.00	49.38
	ATOM	81	C	SER	317	5.696	5.601	18.114	1.00	39.72
	ATOM	82	O	SER	317	6.011	4.446	18.407	1.00	40.21
	ATOM	83	N	ALA	318	6.182	6.220	17.043	1.00	38.35

	ATOM	84	CA	ALA	318	7.114	5.540	16.153	1.00	36.96
	ATOM	85	CB	ALA	318	7.485	6.448	14.986	1.00	37.92
	ATOM	86	C	ALA	318	8.375	5.137	16.920	1.00	38.31
	ATOM	87	O	ALA	318	8.820	3.992	16.844	1.00	33.94
	ATOM	88	N	LEU	319	8.938	6.089	17.664	1.00	36.92
	ATOM	89	CA	LEU	319	10.161	5.854	18.438	1.00	38.56
	ATOM	90	CB	LEU	319	10.660	7.174	19.040	1.00	40.86
	ATOM	91	CG	LEU	319	11.136	8.264	18.071	1.00	41.25
	ATOM	92	CD1	LEU	319	11.714	9.440	18.857	1.00	44.30
	ATOM	93	CD2	LEU	319	12.182	7.693	17.140	1.00	42.61
	ATOM	94	C	LEU	319	9.965	4.826	19.549	1.00	38.33
	ATOM	95	O	LEU	319	10.779	3.916	19.729	1.00	33.91
	ATOM	96	N	LEU	320	8.879	4.982	20.297	1.00	37.39
	ATOM	97	CA	LEU	320	8.567	4.067	21.387	1.00	41.55
	ATOM	98	CB	LEU	320	7.239	4.467	22.049	1.00	38.47
	ATOM	99	CG	LEU	320	7.236	5.582	23.099	1.00	44.81
	ATOM	100	CD1	LEU	320	5.876	5.634	23.802	1.00	44.96
	ATOM	101	CD2	LEU	320	8.334	5.332	24.112	1.00	43.36
	ATOM	102	C	LEU	320	8.466	2.642	20.843	1.00	41.11
	ATOM	103	O	LEU	320	8.971	1.697	21.443	1.00	41.87
	ATOM	104	N	ASP	321	7.812	2.504	19.696	1.00	43.94
	ATOM	105	CA	ASP	321	7.613	1.210	19.053	1.00	44.77
	ATOM	106	CB	ASP	321	6.669	1.372	17.860	1.00	48.39
	ATOM	107	CG	ASP	321	5.206	1.318	18.255	1.00	52.39
	ATOM	108	OD1	ASP	321	4.901	1.422	19.464	1.00	53.56
	ATOM	109	OD2	ASP	321	4.357	1.172	17.346	1.00	55.81
	ATOM	110	C	ASP	321	8.911	0.565	18.568	1.00	44.37
	ATOM	111	O	ASP	321	9.030	-0.661	18.533	1.00	44.67
	ATOM	112	N	ALA	322	9.878	1.395	18.193	1.00	40.75
	ATOM	113	CA	ALA	322	11.153	0.905	17.686	1.00	37.81
	ATOM	114	CB	ALA	322	11.772	1.954	16.776	1.00	38.07
	ATOM	115	C	ALA	322	12.148	0.513	18.769	1.00	35.52
	ATOM	116	O	ALA	322	13.219	-0.020	18.473	1.00	36.11
	ATOM	117	N	GLU	323	11.799	0.768	20.022	1.00	35.61
	ATOM	118	CA	GLU	323	12.704	0.460	21.117	1.00	36.39
	ATOM	119	CB	GLU	323	12.042	0.768	22.459	1.00	35.09
	ATOM	120	CG	GLU	323	12.209	2.210	22.899	1.00	37.93
	ATOM	121	CD	GLU	323	13.657	2.569	23.200	1.00	37.29
	ATOM	122	OE1	GLU	323	14.313	3.173	22.326	1.00	34.21
	ATOM	123	OE2	GLU	323	14.134	2.245	24.309	1.00	38.02
	ATOM	124	C	GLU	323	13.205	-0.978	21.110	1.00	38.01
	ATOM	125	O	GLU	323	12.425	-1.931	20.999	1.00	38.37
	ATOM	126	N	PRO	324	14.527	-1.151	21.225	1.00	36.03
	ATOM	127	CD	PRO	324	15.522	-0.069	21.345	1.00	36.69
	ATOM	128	CA	PRO	324	15.158	-2.474	21.240	1.00	36.42
	ATOM	129	CB	PRO	324	16.633	-2.166	21.003	1.00	35.75
	ATOM	130	CG	PRO	324	16.811	-0.807	21.610	1.00	35.46
	ATOM	131	C	PRO	324	14.940	-3.162	22.583	1.00	35.75

ATOM	132	O	PRO	324	14.616	-2.517	23.580	1.00	34.97
ATOM	133	N	PRO	325	15.134	-4.485	22.631	1.00	35.24
ATOM	134	CD	PRO	325	15.530	-5.386	21.534	1.00	37.02
ATOM	135	CA	PRO	325	14.942	-5.208	23.889	1.00	34.65
ATOM	136	CB	PRO	325	14.753	-6.652	23.439	1.00	35.83
ATOM	137	CG	PRO	325	15.589	-6.743	22.200	1.00	34.88
ATOM	138	C	PRO	325	16.132	-5.070	24.824	1.00	34.51
ATOM	139	O	PRO	325	17.237	-4.723	24.399	1.00	29.92
ATOM	140	N	ILE	326	15.899	-5.322	26.106	1.00	33.62
ATOM	141	CA	ILE	326	16.975	-5.265	27.075	1.00	35.02
ATOM	142	CB	ILE	326	16.458	-4.891	28.473	1.00	38.11
ATOM	143	CG2	ILE	326	17.557	-5.110	29.504	1.00	38.70
ATOM	144	CG1	ILE	326	15.987	-3.431	28.466	1.00	40.48
ATOM	145	CD1	ILE	326	16.035	-2.747	29.815	1.00	42.96
ATOM	146	C	ILE	326	17.567	-6.668	27.103	1.00	34.14
ATOM	147	O	ILE	326	16.875	-7.634	27.427	1.00	34.88
ATOM	148	N	LEU	327	18.840	-6.784	26.745	1.00	29.64
ATOM	149	CA	LEU	327	19.493	-8.083	26.716	1.00	29.54
ATOM	150	CB	LEU	327	20.528	-8.135	25.587	1.00	27.76
ATOM	151	CG	LEU	327	19.978	-7.800	24.196	1.00	29.02
ATOM	152	CD1	LEU	327	21.068	-7.993	23.139	1.00	28.76
ATOM	153	CD2	LEU	327	18.775	-8.688	23.891	1.00	31.26
ATOM	154	C	LEU	327	20.156	-8.438	28.030	1.00	31.21
ATOM	155	O	LEU	327	20.393	-7.578	28.891	1.00	30.12
ATOM	156	N	TYR	328	20.445	-9.725	28.181	1.00	30.99
ATOM	157	CA	TYR	328	21.087	-10.229	29.381	1.00	30.95
ATOM	158	CB	TYR	328	20.409	-11.520	29.842	1.00	33.38
ATOM	159	CG	TYR	328	19.194	-11.272	30.686	1.00	33.05
ATOM	160	CD1	TYR	328	19.253	-11.398	32.071	1.00	31.92
ATOM	161	CE1	TYR	328	18.152	-11.114	32.864	1.00	36.01
ATOM	162	CD2	TYR	328	17.996	-10.862	30.110	1.00	36.05
ATOM	163	CE2	TYR	328	16.880	-10.574	30.899	1.00	37.27
ATOM	164	CZ	TYR	328	16.973	-10.702	32.274	1.00	37.66
ATOM	165	OH	TYR	328	15.896	-10.397	33.071	1.00	44.66
ATOM	166	C	TYR	328	22.529	-10.520	29.067	1.00	33.66
ATOM	167	O	TYR	328	22.884	-10.744	27.910	1.00	34.78
ATOM	168	N	SER	329	23.359	-10.496	30.103	1.00	33.97
ATOM	169	CA	SER	329	24.767	-10.800	29.962	1.00	37.29
ATOM	170	CB	SER	329	25.526	-10.342	31.204	1.00	36.51
ATOM	171	OG	SER	329	26.787	-10.965	31.282	1.00	37.13
ATOM	172	C	SER	329	24.835	-12.317	29.832	1.00	40.43
ATOM	173	O	SER	329	23.980	-13.028	30.363	1.00	40.11
ATOM	174	N	GLU	330	25.845	-12.811	29.128	1.00	41.40
ATOM	175	CA	GLU	330	25.992	-14.242	28.928	1.00	47.43
ATOM	176	CB	GLU	330	26.423	-14.524	27.484	1.00	48.64
ATOM	177	CG	GLU	330	25.278	-14.870	26.542	1.00	50.20
ATOM	178	CD	GLU	330	25.765	-15.405	25.198	1.00	53.25
ATOM	179	OE1	GLU	330	25.909	-16.640	25.062	1.00	53.27

	ATOM	180	OE2	GLU	330	26.004	-14.590	24.280	1.00	51.80
	ATOM	181	C	GLU	330	26.999	-14.852	29.893	1.00	49.67
	ATOM	182	O	GLU	330	28.207	-14.741	29.696	1.00	50.11
	ATOM	183	N	TYR	331	26.498	-15.493	30.942	1.00	53.62
	ATOM	184	CA	TYR	331	27.373	-16.130	31.921	1.00	58.16
	ATOM	185	CB	TYR	331	28.092	-15.078	32.774	1.00	59.55
	ATOM	186	CG	TYR	331	27.239	-14.460	33.860	1.00	63.08
	ATOM	187	CD1	TYR	331	26.656	-13.205	33.682	1.00	64.50
	ATOM	188	CE1	TYR	331	25.864	-12.630	34.676	1.00	65.99
	ATOM	189	CD2	TYR	331	27.010	-15.128	35.065	1.00	63.52
	ATOM	190	CE2	TYR	331	26.219	-14.563	36.066	1.00	65.60
	ATOM	191	CZ	TYR	331	25.648	-13.314	35.864	1.00	67.20
	ATOM	192	OH	TYR	331	24.855	-12.753	36.839	1.00	67.40
	ATOM	193	C	TYR	331	26.603	-17.080	32.823	1.00	59.05
	ATOM	194	O	TYR	331	25.393	-16.942	33.002	1.00	59.22
	ATOM	195	N	ASP	332	27.320	-18.045	33.387	1.00	61.62
	ATOM	196	CA	ASP	332	26.719	-19.026	34.281	1.00	64.20
	ATOM	197	CB	ASP	332	27.681	-20.194	34.500	1.00	65.99
	ATOM	198	CG	ASP	332	26.961	-21.516	34.648	1.00	68.11
	ATOM	199	OD1	ASP	332	27.575	-22.564	34.351	1.00	69.54
	ATOM	200	OD2	ASP	332	25.781	-21.505	35.060	1.00	67.40
	ATOM	201	C	ASP	332	26.393	-18.371	35.619	1.00	63.33
	ATOM	202	O	ASP	332	27.292	-18.073	36.406	1.00	63.90
	ATOM	203	N	PRO	333	25.096	-18.148	35.896	1.00	63.64
	ATOM	204	CD	PRO	333	23.945	-18.509	35.053	1.00	64.35
	ATOM	205	CA	PRO	333	24.677	-17.521	37.154	1.00	63.52
	ATOM	206	CB	PRO	333	23.165	-17.333	36.993	1.00	63.53
	ATOM	207	CG	PRO	333	22.866	-17.611	35.556	1.00	64.15
	ATOM	208	C	PRO	333	25.010	-18.419	38.332	1.00	63.29
	ATOM	209	O	PRO	333	25.129	-17.964	39.468	1.00	63.28
	ATOM	210	N	THR	334	25.160	-19.704	38.037	1.00	64.26
	ATOM	211	CA	THR	334	25.475	-20.697	39.050	1.00	66.09
	ATOM	212	CB	THR	334	24.929	-22.080	38.645	1.00	66.90
	ATOM	213	OG1	THR	334	25.571	-22.513	37.439	1.00	68.06
	ATOM	214	CG2	THR	334	23.423	-22.012	38.411	1.00	67.57
	ATOM	215	C	THR	334	26.982	-20.804	39.269	1.00	65.67
	ATOM	216	O	THR	334	27.432	-21.323	40.289	1.00	64.77
	ATOM	217	N	ARG	335	27.759	-20.308	38.313	1.00	65.65
	ATOM	218	CA	ARG	335	29.214	-20.360	38.421	1.00	66.60
	ATOM	219	CB	ARG	335	29.835	-20.500	37.030	1.00	66.74
	ATOM	220	C	ARG	335	29.757	-19.113	39.123	1.00	67.09
	ATOM	221	O	ARG	335	29.100	-18.071	39.148	1.00	67.31
	ATOM	222	N	PRO	336	30.968	-19.207	39.702	1.00	67.62
	ATOM	223	CD	PRO	336	31.820	-20.408	39.713	1.00	67.30
	ATOM	224	CA	PRO	336	31.601	-18.086	40.410	1.00	67.42
	ATOM	225	CB	PRO	336	32.982	-18.621	40.783	1.00	66.43
	ATOM	226	CG	PRO	336	32.829	-20.097	40.779	1.00	67.52
	ATOM	227	C	PRO	336	31.701	-16.828	39.561	1.00	68.26

ATOM	228	O	PRO	336	31.996	-16.895	38.371	1.00	69.04
ATOM	229	N	PHE	337	31.460	-15.681	40.183	1.00	69.49
ATOM	230	CA	PHE	337	31.529	-14.408	39.480	1.00	71.39
ATOM	231	CB	PHE	337	30.818	-13.323	40.294	1.00	72.31
ATOM	232	CG	PHE	337	31.219	-11.924	39.921	1.00	73.21
ATOM	233	CD1	PHE	337	30.632	-11.287	38.833	1.00	72.82
ATOM	234	CD2	PHE	337	32.191	-11.245	40.653	1.00	73.43
ATOM	235	CE1	PHE	337	31.006	-9.993	38.479	1.00	73.28
ATOM	236	CE2	PHE	337	32.573	-9.950	40.306	1.00	73.00
ATOM	237	CZ	PHE	337	31.980	-9.323	39.217	1.00	72.90
ATOM	238	C	PHE	337	32.985	-14.013	39.245	1.00	71.38
ATOM	239	O	PHE	337	33.336	-13.487	38.189	1.00	71.56
ATOM	240	N	SER	338	33.825	-14.273	40.241	1.00	71.53
ATOM	241	CA	SER	338	35.248	-13.947	40.172	1.00	70.98
ATOM	242	CB	SER	338	35.957	-14.487	41.414	1.00	70.43
ATOM	243	OG	SER	338	35.547	-15.818	41.679	1.00	69.59
ATOM	244	C	SER	338	35.931	-14.504	38.924	1.00	71.20
ATOM	245	O	SER	338	36.951	-13.972	38.475	1.00	71.35
ATOM	246	N	GLU	339	35.368	-15.573	38.369	1.00	70.20
ATOM	247	CA	GLU	339	35.930	-16.215	37.183	1.00	69.48
ATOM	248	CB	GLU	339	35.279	-17.585	36.971	1.00	71.07
ATOM	249	CG	GLU	339	35.996	-18.740	37.656	1.00	72.60
ATOM	250	CD	GLU	339	35.382	-20.089	37.318	1.00	74.26
ATOM	251	OE1	GLU	339	34.786	-20.220	36.227	1.00	73.51
ATOM	252	OE2	GLU	339	35.496	-21.020	38.144	1.00	76.44
ATOM	253	C	GLU	339	35.770	-15.385	35.910	1.00	68.15
ATOM	254	O	GLU	339	36.722	-15.216	35.144	1.00	68.99
ATOM	255	N	ALA	340	34.562	-14.874	35.694	1.00	64.41
ATOM	256	CA	ALA	340	34.246	-14.083	34.507	1.00	60.69
ATOM	257	CB	ALA	340	32.767	-13.709	34.523	1.00	61.17
ATOM	258	C	ALA	340	35.096	-12.824	34.326	1.00	57.00
ATOM	259	O	ALA	340	35.634	-12.270	35.287	1.00	57.46
ATOM	260	N	SER	341	35.215	-12.388	33.076	1.00	52.15
ATOM	261	CA	SER	341	35.972	-11.188	32.736	1.00	46.53
ATOM	262	CB	SER	341	36.839	-11.439	31.497	1.00	48.64
ATOM	263	OG	SER	341	37.184	-10.226	30.846	1.00	46.48
ATOM	264	C	SER	341	34.957	-10.087	32.444	1.00	43.52
ATOM	265	O	SER	341	34.090	-10.248	31.589	1.00	39.92
ATOM	266	N	MET	342	35.052	-8.978	33.166	1.00	41.24
ATOM	267	CA	MET	342	34.121	-7.875	32.960	1.00	42.46
ATOM	268	CB	MET	342	34.449	-6.723	33.912	1.00	45.61
ATOM	269	CG	MET	342	33.228	-6.089	34.560	1.00	52.39
ATOM	270	SD	MET	342	31.791	-7.201	34.631	1.00	57.92
ATOM	271	CE	MET	342	31.999	-7.881	36.239	1.00	56.18
ATOM	272	C	MET	342	34.124	-7.365	31.516	1.00	40.22
ATOM	273	O	MET	342	33.063	-7.121	30.938	1.00	39.23
ATOM	274	N	MET	343	35.307	-7.204	30.930	1.00	38.72
ATOM	275	CA	MET	343	35.395	-6.708	29.558	1.00	38.50

	ATOM	276	CB	MET	343	36.838	-6.318	29.216	1.00	41.15
	ATOM	277	CG	MET	343	37.022	-5.749	27.804	1.00	40.31
	ATOM	278	SD	MET	343	36.032	-4.260	27.427	1.00	45.23
	ATOM	279	CE	MET	343	36.113	-3.358	28.987	1.00	40.45
	ATOM	280	C	MET	343	34.880	-7.741	28.561	1.00	35.36
	ATOM	281	O	MET	343	34.368	-7.384	27.501	1.00	35.51
	ATOM	282	N	GLY	344	35.017	-9.020	28.902	1.00	35.53
	ATOM	283	CA	GLY	344	34.533	-10.072	28.024	1.00	33.41
	ATOM	284	C	GLY	344	33.015	-10.063	28.047	1.00	31.74
	ATOM	285	O	GLY	344	32.359	-10.233	27.019	1.00	29.58
	ATOM	286	N	LEU	345	32.459	-9.860	29.238	1.00	32.89
	ATOM	287	CA	LEU	345	31.011	-9.804	29.415	1.00	34.95
	ATOM	288	CB	LEU	345	30.665	-9.631	30.902	1.00	37.56
	ATOM	289	CG	LEU	345	30.942	-10.774	31.883	1.00	43.03
	ATOM	290	CD1	LEU	345	30.537	-10.357	33.297	1.00	41.57
	ATOM	291	CD2	LEU	345	30.164	-11.998	31.449	1.00	42.80
	ATOM	292	C	LEU	345	30.430	-8.614	28.633	1.00	33.71
	ATOM	293	O	LEU	345	29.479	-8.757	27.868	1.00	30.29
	ATOM	294	N	LEU	346	31.021	-7.443	28.843	1.00	30.20
	ATOM	295	CA	LEU	346	30.569	-6.217	28.193	1.00	32.00
	ATOM	296	CB	LEU	346	31.317	-5.016	28.771	1.00	28.16
	ATOM	297	CG	LEU	346	31.091	-4.767	30.269	1.00	29.84
	ATOM	298	CD1	LEU	346	31.815	-3.498	30.668	1.00	29.98
	ATOM	299	CD2	LEU	346	29.614	-4.644	30.581	1.00	33.97
	ATOM	300	C	LEU	346	30.732	-6.250	26.682	1.00	30.70
	ATOM	301	O	LEU	346	29.869	-5.765	25.955	1.00	29.13
	ATOM	302	N	THR	347	31.839	-6.816	26.212	1.00	30.47
	ATOM	303	CA	THR	347	32.086	-6.911	24.781	1.00	30.93
	ATOM	304	CB	THR	347	33.472	-7.501	24.497	1.00	29.97
	ATOM	305	OG1	THR	347	34.481	-6.604	24.982	1.00	35.40
	ATOM	306	CG2	THR	347	33.666	-7.707	23.004	1.00	33.58
	ATOM	307	C	THR	347	31.036	-7.804	24.122	1.00	31.97
	ATOM	308	O	THR	347	30.516	-7.486	23.049	1.00	30.75
	ATOM	309	N	ASN	348	30.737	-8.926	24.768	1.00	29.31
	ATOM	310	CA	ASN	348	29.757	-9.868	24.242	1.00	32.63
	ATOM	311	CB	ASN	348	29.767	-11.161	25.065	1.00	31.64
	ATOM	312	CG	ASN	348	28.646	-12.117	24.662	1.00	39.14
	ATOM	313	OD1	ASN	348	27.549	-12.078	25.220	1.00	41.91
	ATOM	314	ND2	ASN	348	28.920	-12.970	23.683	1.00	42.05
	ATOM	315	C	ASN	348	28.361	-9.251	24.262	1.00	29.02
	ATOM	316	O	ASN	348	27.558	-9.477	23.353	1.00	32.76
	ATOM	317	N	LEU	349	28.078	-8.467	25.298	1.00	28.74
	ATOM	318	CA	LEU	349	26.782	-7.811	25.421	1.00	28.58
	ATOM	319	CB	LEU	349	26.650	-7.148	26.795	1.00	26.56
	ATOM	320	CG	LEU	349	25.376	-6.328	27.050	1.00	33.67
	ATOM	321	CD1	LEU	349	24.140	-7.199	26.840	1.00	28.82
	ATOM	322	CD2	LEU	349	25.392	-5.779	28.471	1.00	33.11
	ATOM	323	C	LEU	349	26.638	-6.762	24.319	1.00	28.07

	ATOM	324	O	LEU	349	25.616	-6.703	23.629	1.00	25.22
	ATOM	325	N	ALA	350	27.675	-5.941	24.157	1.00	28.50
	ATOM	326	CA	ALA	350	27.668	-4.886	23.148	1.00	28.46
	ATOM	327	CB	ALA	350	28.972	-4.094	23.209	1.00	28.12
	ATOM	328	C	ALA	350	27.468	-5.461	21.750	1.00	28.75
	ATOM	329	O	ALA	350	26.649	-4.958	20.983	1.00	30.90
	ATOM	330	N	ASP	351	28.213	-6.509	21.420	1.00	27.20
	ATOM	331	CA	ASP	351	28.093	-7.143	20.112	1.00	29.75
	ATOM	332	CB	ASP	351	29.036	-8.345	20.010	1.00	34.16
	ATOM	333	CG	ASP	351	30.498	-7.940	19.978	1.00	37.50
	ATOM	334	OD1	ASP	351	31.354	-8.831	20.148	1.00	37.55
	ATOM	335	OD2	ASP	351	30.789	-6.738	19.784	1.00	35.50
	ATOM	336	C	ASP	351	26.661	-7.600	19.813	1.00	30.52
	ATOM	337	O	ASP	351	26.193	-7.458	18.687	1.00	27.77
	ATOM	338	N	ARG	352	25.968	-8.150	20.811	1.00	27.18
	ATOM	339	CA	ARG	352	24.593	-8.602	20.605	1.00	26.21
	ATOM	340	CB	ARG	352	24.148	-9.534	21.752	1.00	26.52
	ATOM	341	CG	ARG	352	24.567	-10.991	21.532	1.00	31.03
	ATOM	342	CD	ARG	352	24.128	-11.911	22.666	1.00	29.80
	ATOM	343	NE	ARG	352	24.898	-11.675	23.879	1.00	30.44
	ATOM	344	CZ	ARG	352	24.364	-11.363	25.054	1.00	31.68
	ATOM	345	NH1	ARG	352	23.050	-11.251	25.177	1.00	31.18
	ATOM	346	NH2	ARG	352	25.144	-11.148	26.104	1.00	32.03
	ATOM	347	C	ARG	352	23.642	-7.411	20.502	1.00	27.16
	ATOM	348	O	ARG	352	22.702	-7.426	19.708	1.00	26.65
	ATOM	349	N	GLU	353	23.896	-6.370	21.291	1.00	24.30
	ATOM	350	CA	GLU	353	23.045	-5.178	21.261	1.00	26.39
	ATOM	351	CB	GLU	353	23.461	-4.204	22.365	1.00	24.91
	ATOM	352	CG	GLU	353	23.147	-4.669	23.771	1.00	27.93
	ATOM	353	CD	GLU	353	23.425	-3.587	24.795	1.00	30.71
	ATOM	354	OE1	GLU	353	24.564	-3.534	25.304	1.00	30.09
	ATOM	355	OE2	GLU	353	22.506	-2.789	25.085	1.00	30.53
	ATOM	356	C	GLU	353	23.131	-4.456	19.920	1.00	24.27
	ATOM	357	O	GLU	353	22.169	-3.826	19.467	1.00	28.71
	ATOM	358	N	LEU	354	24.296	-4.540	19.293	1.00	26.61
	ATOM	359	CA	LEU	354	24.522	-3.872	18.017	1.00	26.62
	ATOM	360	CB	LEU	354	25.952	-4.121	17.543	1.00	26.36
	ATOM	361	CG	LEU	354	26.372	-3.257	16.351	1.00	29.24
	ATOM	362	CD1	LEU	354	26.243	-1.774	16.722	1.00	26.59
	ATOM	363	CD2	LEU	354	27.794	-3.607	15.962	1.00	28.88
	ATOM	364	C	LEU	354	23.559	-4.300	16.926	1.00	27.72
	ATOM	365	O	LEU	354	23.074	-3.475	16.152	1.00	24.00
	ATOM	366	N	VAL	355	23.291	-5.598	16.854	1.00	28.82
	ATOM	367	CA	VAL	355	22.386	-6.125	15.844	1.00	29.45
	ATOM	368	CB	VAL	355	22.259	-7.655	15.975	1.00	31.76
	ATOM	369	CG1	VAL	355	21.423	-8.205	14.834	1.00	33.55
	ATOM	370	CG2	VAL	355	23.649	-8.282	15.998	1.00	31.36
	ATOM	371	C	VAL	355	21.020	-5.499	16.035	1.00	27.71

	ATOM	372	O	VAL	355	20.382	-5.039	15.080	1.00	29.61
	ATOM	373	N	HIS	356	20.580	-5.473	17.288	1.00	27.76
	ATOM	374	CA	HIS	356	19.291	-4.906	17.627	1.00	28.35
	ATOM	375	CB	HIS	356	18.936	-5.231	19.079	1.00	31.12
5	ATOM	376	CG	HIS	356	18.602	-6.675	19.307	1.00	35.93
	ATOM	377	CD2	HIS	356	19.352	-7.700	19.779	1.00	33.95
	ATOM	378	ND1	HIS	356	17.363	-7.208	19.018	1.00	36.62
	ATOM	379	CE1	HIS	356	17.364	-8.499	19.304	1.00	33.33
	ATOM	380	NE2	HIS	356	18.559	-8.823	19.767	1.00	32.16
10	ATOM	381	C	HIS	356	19.300	-3.398	17.412	1.00	28.25
	ATOM	382	O	HIS	356	18.272	-2.812	17.100	1.00	28.99
	ATOM	383	N	MET	357	20.457	-2.765	17.574	1.00	25.31
	ATOM	384	CA	MET	357	20.526	-1.322	17.369	1.00	24.63
	ATOM	385	CB	MET	357	21.902	-0.789	17.766	1.00	23.61
15	ATOM	386	CG	MET	357	22.011	0.736	17.699	1.00	24.66
	ATOM	387	SD	MET	357	23.732	1.290	17.859	1.00	27.30
	ATOM	388	CE	MET	357	24.140	0.672	19.514	1.00	23.62
	ATOM	389	C	MET	357	20.256	-1.011	15.898	1.00	24.83
	ATOM	390	O	MET	357	19.619	-0.003	15.569	1.00	26.78
20	ATOM	391	N	ILE	358	20.757	-1.874	15.020	1.00	26.25
	ATOM	392	CA	ILE	358	20.553	-1.721	13.576	1.00	30.33
	ATOM	393	CB	ILE	358	21.204	-2.888	12.789	1.00	33.86
	ATOM	394	CG2	ILE	358	20.759	-2.860	11.334	1.00	33.68
	ATOM	395	CG1	ILE	358	22.728	-2.799	12.874	1.00	36.89
25	ATOM	396	CD1	ILE	358	23.299	-1.469	12.451	1.00	39.10
	ATOM	397	C	ILE	358	19.055	-1.721	13.310	1.00	32.20
	ATOM	398	O	ILE	358	18.519	-0.817	12.662	1.00	32.02
	ATOM	399	N	ASN	359	18.379	-2.748	13.814	1.00	33.12
	ATOM	400	CA	ASN	359	16.945	-2.861	13.638	1.00	33.35
30	ATOM	401	CB	ASN	359	16.434	-4.101	14.363	1.00	37.59
	ATOM	402	CG	ASN	359	16.739	-5.374	13.627	1.00	44.38
	ATOM	403	OD1	ASN	359	17.045	-5.329	12.437	1.00	47.35
	ATOM	404	ND2	ASN	359	16.673	-6.508	14.320	1.00	42.48
	ATOM	405	C	ASN	359	16.224	-1.634	14.149	1.00	32.74
35	ATOM	406	O	ASN	359	15.261	-1.163	13.530	1.00	31.39
	ATOM	407	N	TRP	360	16.706	-1.104	15.264	1.00	27.92
	ATOM	408	CA	TRP	360	16.102	0.087	15.842	1.00	29.47
	ATOM	409	CB	TRP	360	16.703	0.347	17.228	1.00	27.66
	ATOM	410	CG	TRP	360	16.522	1.747	17.707	1.00	30.40
40	ATOM	411	CD2	TRP	360	17.493	2.801	17.657	1.00	27.54
	ATOM	412	CE2	TRP	360	16.888	3.954	18.204	1.00	29.42
	ATOM	413	CE3	TRP	360	18.819	2.883	17.205	1.00	28.37
	ATOM	414	CD1	TRP	360	15.399	2.284	18.264	1.00	27.75
	ATOM	415	NE1	TRP	360	15.609	3.611	18.566	1.00	30.84
45	ATOM	416	CZ2	TRP	360	17.558	5.180	18.310	1.00	27.74
	ATOM	417	CZ3	TRP	360	19.488	4.106	17.309	1.00	24.49
	ATOM	418	CH2	TRP	360	18.853	5.232	17.858	1.00	25.09
	ATOM	419	C	TRP	360	16.312	1.296	14.926	1.00	27.90

	ATOM	420	O	TRP	360	15.360	2.002	14.581	1.00	28.83
	ATOM	421	N	ALA	361	17.559	1.520	14.523	1.00	28.25
	ATOM	422	CA	ALA	361	17.894	2.637	13.645	1.00	29.20
	ATOM	423	CB	ALA	361	19.346	2.539	13.220	1.00	28.89
	ATOM	424	C	ALA	361	17.006	2.685	12.403	1.00	31.08
	ATOM	425	O	ALA	361	16.531	3.746	12.011	1.00	31.30
	ATOM	426	N	LYS	362	16.795	1.526	11.783	1.00	30.93
	ATOM	427	CA	LYS	362	15.981	1.443	10.581	1.00	34.15
	ATOM	428	CB	LYS	362	16.012	0.016	10.023	1.00	33.67
	ATOM	429	CG	LYS	362	17.252	-0.281	9.198	1.00	39.40
	ATOM	430	CD	LYS	362	17.547	-1.774	9.136	1.00	43.60
	ATOM	431	CE	LYS	362	18.852	-2.046	8.389	1.00	47.06
	ATOM	432	NZ	LYS	362	19.178	-3.507	8.288	1.00	50.34
	ATOM	433	C	LYS	362	14.545	1.872	10.815	1.00	35.81
	ATOM	434	O	LYS	362	13.821	2.168	9.859	1.00	37.95
	ATOM	435	N	ARG	363	14.134	1.921	12.079	1.00	34.23
	ATOM	436	CA	ARG	363	12.770	2.313	12.409	1.00	36.04
	ATOM	437	CB	ARG	363	12.178	1.307	13.391	1.00	36.71
	ATOM	438	CG	ARG	363	12.169	-0.110	12.827	1.00	40.36
	ATOM	439	CD	ARG	363	11.468	-1.086	13.746	1.00	42.17
	ATOM	440	NE	ARG	363	10.161	-0.586	14.158	1.00	45.19
	ATOM	441	CZ	ARG	363	9.314	-1.262	14.929	1.00	49.41
	ATOM	442	NH1	ARG	363	9.642	-2.467	15.374	1.00	48.02
	ATOM	443	NH2	ARG	363	8.143	-0.729	15.261	1.00	51.54
	ATOM	444	C	ARG	363	12.654	3.743	12.943	1.00	37.40
	ATOM	445	O	ARG	363	11.567	4.199	13.303	1.00	38.22
	ATOM	446	N	VAL	364	13.785	4.442	13.002	1.00	35.66
	ATOM	447	CA	VAL	364	13.804	5.836	13.431	1.00	34.06
	ATOM	448	CB	VAL	364	15.231	6.271	13.827	1.00	33.87
	ATOM	449	CG1	VAL	364	15.293	7.779	13.995	1.00	31.08
	ATOM	450	CG2	VAL	364	15.641	5.571	15.113	1.00	31.30
	ATOM	451	C	VAL	364	13.360	6.591	12.171	1.00	33.19
	ATOM	452	O	VAL	364	14.028	6.531	11.146	1.00	33.04
	ATOM	453	N	PRO	365	12.225	7.310	12.234	1.00	34.69
	ATOM	454	CD	PRO	365	11.359	7.492	13.413	1.00	34.19
	ATOM	455	CA	PRO	365	11.724	8.050	11.069	1.00	35.96
	ATOM	456	CB	PRO	365	10.608	8.918	11.645	1.00	36.59
	ATOM	457	CG	PRO	365	10.135	8.157	12.842	1.00	39.59
	ATOM	458	C	PRO	365	12.756	8.878	10.321	1.00	37.19
	ATOM	459	O	PRO	365	13.430	9.726	10.907	1.00	40.29
	ATOM	460	N	GLY	366	12.878	8.624	9.023	1.00	34.78
	ATOM	461	CA	GLY	366	13.816	9.371	8.212	1.00	33.54
	ATOM	462	C	GLY	366	15.168	8.722	8.007	1.00	34.26
	ATOM	463	O	GLY	366	15.858	9.035	7.034	1.00	37.15
	ATOM	464	N	PHE	367	15.554	7.814	8.901	1.00	33.13
	ATOM	465	CA	PHE	367	16.860	7.164	8.787	1.00	32.04
	ATOM	466	CB	PHE	367	17.138	6.291	10.016	1.00	30.22
	ATOM	467	CG	PHE	367	18.544	5.773	10.080	1.00	30.60

	ATOM	468	CD1	PHE	367	18.827	4.446	9.751	1.00	31.94
	ATOM	469	CD2	PHE	367	19.589	6.601	10.485	1.00	29.20
	ATOM	470	CE1	PHE	367	20.133	3.950	9.828	1.00	28.30
	ATOM	471	CE2	PHE	367	20.896	6.122	10.568	1.00	28.12
	ATOM	472	CZ	PHE	367	21.171	4.791	10.240	1.00	25.41
	ATOM	473	C	PHE	367	17.033	6.333	7.524	1.00	31.46
	ATOM	474	O	PHE	367	18.073	6.405	6.883	1.00	32.30
	ATOM	475	N	VAL	368	16.027	5.541	7.165	1.00	35.20
	ATOM	476	CA	VAL	368	16.123	4.718	5.959	1.00	38.98
	ATOM	477	CB	VAL	368	15.076	3.584	5.945	1.00	40.61
	ATOM	478	CG1	VAL	368	15.543	2.447	6.843	1.00	41.48
	ATOM	479	CG2	VAL	368	13.717	4.113	6.390	1.00	41.60
	ATOM	480	C	VAL	368	15.965	5.523	4.673	1.00	40.06
	ATOM	481	O	VAL	368	16.156	4.992	3.579	1.00	41.66
	ATOM	482	N	ASP	369	15.608	6.798	4.798	1.00	38.65
	ATOM	483	CA	ASP	369	15.465	7.646	3.621	1.00	37.15
	ATOM	484	CB	ASP	369	14.700	8.929	3.954	1.00	39.89
	ATOM	485	CG	ASP	369	13.254	8.671	4.302	1.00	45.59
	ATOM	486	OD1	ASP	369	12.686	7.672	3.806	1.00	46.34
	ATOM	487	OD2	ASP	369	12.681	9.472	5.074	1.00	49.13
	ATOM	488	C	ASP	369	16.855	8.010	3.136	1.00	34.91
	ATOM	489	O	ASP	369	17.038	8.431	1.995	1.00	34.25
	ATOM	490	N	LEU	370	17.838	7.841	4.016	1.00	31.76
	ATOM	491	CA	LEU	370	19.229	8.153	3.705	1.00	28.08
	ATOM	492	CB	LEU	370	20.020	8.339	5.003	1.00	28.81
	ATOM	493	CG	LEU	370	19.523	9.395	6.000	1.00	28.74
	ATOM	494	CD1	LEU	370	20.315	9.275	7.299	1.00	30.81
	ATOM	495	CD2	LEU	370	19.693	10.792	5.404	1.00	29.77
	ATOM	496	C	LEU	370	19.884	7.043	2.893	1.00	31.25
	ATOM	497	O	LEU	370	19.341	5.943	2.784	1.00	31.78
	ATOM	498	N	THR	371	21.052	7.333	2.331	1.00	28.86
	ATOM	499	CA	THR	371	21.793	6.336	1.569	1.00	32.90
	ATOM	500	CB	THR	371	22.979	6.944	0.818	1.00	33.44
	ATOM	501	OG1	THR	371	23.880	7.523	1.766	1.00	34.59
	ATOM	502	CG2	THR	371	22.514	8.002	-0.178	1.00	32.63
	ATOM	503	C	THR	371	22.373	5.315	2.539	1.00	35.31
	ATOM	504	O	THR	371	22.536	5.591	3.733	1.00	31.27
	ATOM	505	N	LEU	372	22.702	4.141	2.015	1.00	34.34
	ATOM	506	CA	LEU	372	23.273	3.073	2.822	1.00	35.46
	ATOM	507	CB	LEU	372	23.518	1.841	1.944	1.00	37.73
	ATOM	508	CG	LEU	372	24.362	0.704	2.515	1.00	42.43
	ATOM	509	CD1	LEU	372	23.690	0.145	3.757	1.00	45.60
	ATOM	510	CD2	LEU	372	24.534	-0.383	1.455	1.00	44.29
	ATOM	511	C	LEU	372	24.587	3.548	3.444	1.00	36.95
	ATOM	512	O	LEU	372	24.813	3.374	4.643	1.00	35.57
	ATOM	513	N	HIS	373	25.442	4.159	2.627	1.00	35.68
	ATOM	514	CA	HIS	373	26.729	4.656	3.099	1.00	36.60
	ATOM	515	CB	HIS	373	27.506	5.282	1.935	1.00	44.01

ATOM	516	CG	HIS	373	28.538	6.280	2.360	1.00	50.69
ATOM	517	CD2	HIS	373	29.857	6.138	2.636	1.00	54.69
ATOM	518	ND1	HIS	373	28.246	7.613	2.561	1.00	53.77
ATOM	519	CE1	HIS	373	29.339	8.248	2.945	1.00	57.09
ATOM	520	NE2	HIS	373	30.331	7.376	2.999	1.00	57.23
ATOM	521	C	HIS	373	26.575	5.669	4.244	1.00	36.22
ATOM	522	O	HIS	373	27.350	5.650	5.201	1.00	33.05
ATOM	523	N	ASP	374	25.580	6.549	4.148	1.00	32.03
ATOM	524	CA	ASP	374	25.342	7.541	5.196	1.00	30.76
ATOM	525	CB	ASP	374	24.354	8.603	4.713	1.00	30.12
ATOM	526	CG	ASP	374	25.018	9.672	3.860	1.00	35.83
ATOM	527	OD1	ASP	374	26.264	9.744	3.842	1.00	34.39
ATOM	528	OD2	ASP	374	24.291	10.440	3.199	1.00	35.39
ATOM	529	C	ASP	374	24.805	6.876	6.472	1.00	30.33
ATOM	530	O	ASP	374	25.152	7.275	7.587	1.00	27.04
ATOM	531	N	GLN	375	23.944	5.877	6.309	1.00	25.71
ATOM	532	CA	GLN	375	23.403	5.157	7.454	1.00	26.68
ATOM	533	CB	GLN	375	22.424	4.077	6.993	1.00	29.70
ATOM	534	CG	GLN	375	21.101	4.616	6.484	1.00	29.16
ATOM	535	CD	GLN	375	20.219	3.514	5.940	1.00	35.87
ATOM	536	OE1	GLN	375	20.155	2.426	6.510	1.00	30.97
ATOM	537	NE2	GLN	375	19.541	3.785	4.827	1.00	34.51
ATOM	538	C	GLN	375	24.556	4.502	8.214	1.00	25.51
ATOM	539	O	GLN	375	24.585	4.513	9.442	1.00	28.14
ATOM	540	N	VAL	376	25.504	3.938	7.475	1.00	26.62
ATOM	541	CA	VAL	376	26.659	3.281	8.071	1.00	29.24
ATOM	542	CB	VAL	376	27.531	2.597	7.003	1.00	29.66
ATOM	543	CG1	VAL	376	28.812	2.071	7.635	1.00	28.29
ATOM	544	CG2	VAL	376	26.745	1.469	6.341	1.00	29.90
ATOM	545	C	VAL	376	27.526	4.285	8.821	1.00	30.87
ATOM	546	O	VAL	376	27.953	4.029	9.948	1.00	30.09
ATOM	547	N	HIS	377	27.785	5.428	8.191	1.00	28.05
ATOM	548	CA	HIS	377	28.602	6.457	8.814	1.00	28.68
ATOM	549	CB	HIS	377	28.792	7.639	7.864	1.00	30.26
ATOM	550	CG	HIS	377	29.508	8.791	8.488	1.00	33.89
ATOM	551	CD2	HIS	377	29.073	10.017	8.863	1.00	34.99
ATOM	552	ND1	HIS	377	30.846	8.740	8.823	1.00	37.01
ATOM	553	CE1	HIS	377	31.201	9.884	9.377	1.00	34.79
ATOM	554	NE2	HIS	377	30.144	10.677	9.413	1.00	34.95
ATOM	555	C	HIS	377	27.983	6.954	10.114	1.00	25.13
ATOM	556	O	HIS	377	28.677	7.102	11.115	1.00	25.93
ATOM	557	N	LEU	378	26.678	7.206	10.107	1.00	24.58
ATOM	558	CA	LEU	378	26.015	7.695	11.315	1.00	26.40
ATOM	559	CB	LEU	378	24.542	8.001	11.027	1.00	26.29
ATOM	560	CG	LEU	378	24.291	9.180	10.073	1.00	28.06
ATOM	561	CD1	LEU	378	22.778	9.353	9.869	1.00	27.66
ATOM	562	CD2	LEU	378	24.911	10.458	10.642	1.00	30.08
ATOM	563	C	LEU	378	26.120	6.695	12.459	1.00	28.55

ATOM	564	O	LEU	378	26.379	7.075	13.605	1.00	24.76
ATOM	565	N	LEU	379	25.919	5.414	12.153	1.00	24.29
ATOM	566	CA	LEU	379	26.000	4.388	13.182	1.00	27.03
ATOM	567	CB	LEU	379	25.401	3.073	12.667	1.00	28.53
ATOM	568	CG	LEU	379	23.875	3.023	12.845	1.00	30.29
ATOM	569	CD1	LEU	379	23.248	1.943	11.963	1.00	33.04
ATOM	570	CD2	LEU	379	23.563	2.759	14.312	1.00	29.45
ATOM	571	C	LEU	379	27.430	4.176	13.670	1.00	27.18
ATOM	572	O	LEU	379	27.653	3.979	14.866	1.00	25.95
ATOM	573	N	GLU	380	28.402	4.236	12.762	1.00	25.86
ATOM	574	CA	GLU	380	29.786	4.054	13.173	1.00	27.58
ATOM	575	CB	GLU	380	30.730	4.036	11.968	1.00	30.36
ATOM	576	CG	GLU	380	32.172	3.785	12.380	1.00	37.98
ATOM	577	CD	GLU	380	33.080	3.471	11.210	1.00	45.23
ATOM	578	OE1	GLU	380	32.869	4.048	10.120	1.00	42.99
ATOM	579	OE2	GLU	380	34.004	2.646	11.386	1.00	45.79
ATOM	580	C	GLU	380	30.218	5.159	14.133	1.00	27.50
ATOM	581	O	GLU	380	31.056	4.937	15.010	1.00	26.67
ATOM	582	N	ACYS	381	29.637	6.339	13.965	0.75	24.89
ATOM	583	N	BCYS	381	29.645	6.352	13.980	0.25	25.79
ATOM	584	CA	ACYS	381	29.969	7.466	14.826	0.75	24.12
ATOM	585	CA	BCYS	381	29.993	7.481	14.847	0.25	24.86
ATOM	586	CB	ACYS	381	29.621	8.781	14.122	0.75	25.96
ATOM	587	CB	BCYS	381	29.766	8.814	14.115	0.25	25.62
ATOM	588	SG	ACYS	381	30.698	9.192	12.732	0.75	31.63
ATOM	589	SG	BCYS	381	30.227	10.312	15.059	0.25	25.40
ATOM	590	C	ACYS	381	29.237	7.422	16.162	0.75	22.07
ATOM	591	C	BCYS	381	29.211	7.498	16.159	0.25	23.97
ATOM	592	O	ACYS	381	29.812	7.730	17.206	0.75	21.97
ATOM	593	O	BCYS	381	29.724	7.940	17.187	0.25	23.99
ATOM	594	N	ALA	382	27.974	7.012	16.128	1.00	23.41
ATOM	595	CA	ALA	382	27.140	7.015	17.318	1.00	22.83
ATOM	596	CB	ALA	382	25.785	7.587	16.948	1.00	25.50
ATOM	597	C	ALA	382	26.913	5.755	18.131	1.00	25.39
ATOM	598	O	ALA	382	26.374	5.837	19.234	1.00	23.09
ATOM	599	N	TRP	383	27.311	4.602	17.615	1.00	25.98
ATOM	600	CA	TRP	383	27.026	3.354	18.318	1.00	23.80
ATOM	601	CB	TRP	383	27.669	2.172	17.580	1.00	22.52
ATOM	602	CG	TRP	383	29.130	2.054	17.762	1.00	24.42
ATOM	603	CD2	TRP	383	29.797	1.347	18.803	1.00	27.31
ATOM	604	CE2	TRP	383	31.182	1.484	18.579	1.00	28.24
ATOM	605	CE3	TRP	383	29.360	0.609	19.912	1.00	27.37
ATOM	606	CD1	TRP	383	30.102	2.578	16.965	1.00	24.58
ATOM	607	NE1	TRP	383	31.342	2.239	17.446	1.00	27.35
ATOM	608	CZ2	TRP	383	32.133	0.909	19.420	1.00	28.76
ATOM	609	CZ3	TRP	383	30.305	0.039	20.745	1.00	28.09
ATOM	610	CH2	TRP	383	31.674	0.191	20.496	1.00	29.77
ATOM	611	C	TRP	383	27.356	3.309	19.802	1.00	23.54

	ATOM	612	O	TRP	383	26.526	2.866	20.584	1.00	22.90
	ATOM	613	N	LEU	384	28.542	3.765	20.211	1.00	20.37
	ATOM	614	CA	LEU	384	28.864	3.713	21.640	1.00	22.41
	ATOM	615	CB	LEU	384	30.369	3.890	21.883	1.00	24.98
5	ATOM	616	CG	LEU	384	30.824	3.645	23.336	1.00	27.33
	ATOM	617	CD1	LEU	384	30.273	2.305	23.853	1.00	29.71
	ATOM	618	CD2	LEU	384	32.336	3.648	23.398	1.00	26.07
	ATOM	619	C	LEU	384	28.075	4.732	22.453	1.00	19.44
	ATOM	620	O	LEU	384	27.706	4.458	23.595	1.00	23.24
10	ATOM	621	N	GLU	385	27.807	5.909	21.885	1.00	20.80
	ATOM	622	CA	GLU	385	27.011	6.895	22.612	1.00	21.32
	ATOM	623	CB	GLU	385	26.861	8.177	21.797	1.00	21.91
	ATOM	624	CG	GLU	385	28.115	9.020	21.705	1.00	21.61
	ATOM	625	CD	GLU	385	27.882	10.256	20.860	1.00	29.53
15	ATOM	626	OE1	GLU	385	27.374	11.256	21.401	1.00	30.54
	ATOM	627	OE2	GLU	385	28.188	10.219	19.658	1.00	29.97
	ATOM	628	C	GLU	385	25.616	6.292	22.836	1.00	22.26
	ATOM	629	O	GLU	385	25.022	6.438	23.902	1.00	22.26
	ATOM	630	N	ILE	386	25.101	5.617	21.812	1.00	22.03
20	ATOM	631	CA	ILE	386	23.779	4.995	21.896	1.00	22.74
	ATOM	632	CB	ILE	386	23.328	4.455	20.498	1.00	22.88
	ATOM	633	CG2	ILE	386	22.009	3.647	20.618	1.00	23.85
	ATOM	634	CG1	ILE	386	23.085	5.651	19.561	1.00	25.05
	ATOM	635	CD1	ILE	386	22.994	5.297	18.078	1.00	26.42
25	ATOM	636	C	ILE	386	23.766	3.897	22.961	1.00	22.50
	ATOM	637	O	ILE	386	22.823	3.818	23.746	1.00	24.75
	ATOM	638	N	LEU	387	24.810	3.071	23.020	1.00	22.25
	ATOM	639	CA	LEU	387	24.868	2.030	24.051	1.00	22.95
	ATOM	640	CB	LEU	387	26.096	1.132	23.864	1.00	24.61
30	ATOM	641	CG	LEU	387	26.070	0.194	22.654	1.00	23.21
	ATOM	642	CD1	LEU	387	27.297	-0.709	22.705	1.00	25.36
	ATOM	643	CD2	LEU	387	24.791	-0.631	22.652	1.00	26.29
	ATOM	644	C	LEU	387	24.944	2.660	25.438	1.00	26.22
	ATOM	645	O	LEU	387	24.287	2.204	26.386	1.00	23.55
35	ATOM	646	N	MET	388	25.751	3.713	25.554	1.00	23.92
	ATOM	647	CA	MET	388	25.924	4.385	26.835	1.00	24.26
	ATOM	648	CB	MET	388	27.088	5.378	26.761	1.00	23.87
	ATOM	649	CG	MET	388	28.440	4.722	26.743	1.00	24.08
	ATOM	650	SD	MET	388	29.726	5.992	26.736	1.00	27.70
40	ATOM	651	CE	MET	388	31.139	5.041	27.078	1.00	21.74
	ATOM	652	C	MET	388	24.660	5.094	27.321	1.00	23.33
	ATOM	653	O	MET	388	24.341	5.026	28.505	1.00	25.58
	ATOM	654	N	ILE	389	23.935	5.775	26.436	1.00	24.62
	ATOM	655	CA	ILE	389	22.729	6.440	26.905	1.00	24.03
45	ATOM	656	CB	ILE	389	22.132	7.439	25.852	1.00	27.01
	ATOM	657	CG2	ILE	389	21.413	6.705	24.706	1.00	23.98
	ATOM	658	CG1	ILE	389	21.185	8.402	26.584	1.00	25.49
	ATOM	659	CD1	ILE	389	20.431	9.383	25.683	1.00	25.45

ATOM	660	C	ILE	389	21.694	5.401	27.349	1.00	26.54
ATOM	661	O	ILE	389	20.938	5.631	28.294	1.00	22.58
ATOM	662	N	GLY	390	21.679	4.247	26.687	1.00	27.14
ATOM	663	CA	GLY	390	20.753	3.201	27.090	1.00	28.42
ATOM	664	C	GLY	390	21.133	2.719	28.482	1.00	29.67
ATOM	665	O	GLY	390	20.275	2.521	29.348	1.00	29.21
ATOM	666	N	LEU	391	22.433	2.547	28.699	1.00	26.06
ATOM	667	CA	LEU	391	22.955	2.091	29.983	1.00	29.23
ATOM	668	CB	LEU	391	24.476	1.937	29.899	1.00	28.37
ATOM	669	CG	LEU	391	25.206	1.656	31.210	1.00	30.81
ATOM	670	CD1	LEU	391	24.717	0.332	31.793	1.00	25.73
ATOM	671	CD2	LEU	391	26.709	1.619	30.958	1.00	25.25
ATOM	672	C	LEU	391	22.603	3.070	31.104	1.00	30.84
ATOM	673	O	LEU	391	22.156	2.669	32.186	1.00	29.19
ATOM	674	N	VAL	392	22.817	4.355	30.850	1.00	28.91
ATOM	675	CA	VAL	392	22.506	5.369	31.851	1.00	28.86
ATOM	676	CB	VAL	392	22.923	6.770	31.353	1.00	30.08
ATOM	677	CG1	VAL	392	22.329	7.854	32.237	1.00	32.32
ATOM	678	CG2	VAL	392	24.442	6.870	31.372	1.00	28.52
ATOM	679	C	VAL	392	21.013	5.327	32.165	1.00	28.42
ATOM	680	O	VAL	392	20.621	5.345	33.327	1.00	30.38
ATOM	681	N	TRP	393	20.191	5.241	31.125	1.00	28.23
ATOM	682	CA	TRP	393	18.732	5.186	31.280	1.00	29.70
ATOM	683	CB	TRP	393	18.066	5.046	29.906	1.00	30.09
ATOM	684	CG	TRP	393	16.605	4.670	29.953	1.00	33.50
ATOM	685	CD2	TRP	393	15.516	5.499	30.369	1.00	31.76
ATOM	686	CE2	TRP	393	14.336	4.725	30.264	1.00	38.11
ATOM	687	CE3	TRP	393	15.419	6.821	30.824	1.00	32.56
ATOM	688	CD1	TRP	393	16.057	3.459	29.618	1.00	34.31
ATOM	689	NE1	TRP	393	14.696	3.486	29.801	1.00	34.36
ATOM	690	CZ2	TRP	393	13.073	5.233	30.597	1.00	37.93
ATOM	691	CZ3	TRP	393	14.162	7.326	31.155	1.00	35.24
ATOM	692	CH2	TRP	393	13.007	6.531	31.039	1.00	37.77
ATOM	693	C	TRP	393	18.256	4.051	32.191	1.00	32.07
ATOM	694	O	TRP	393	17.460	4.275	33.109	1.00	32.12
ATOM	695	N	ARG	394	18.738	2.837	31.957	1.00	31.90
ATOM	696	CA	ARG	394	18.288	1.729	32.787	1.00	36.63
ATOM	697	CB	ARG	394	18.492	0.389	32.065	1.00	36.41
ATOM	698	CG	ARG	394	19.914	0.009	31.764	1.00	36.50
ATOM	699	CD	ARG	394	19.929	-1.132	30.748	1.00	36.34
ATOM	700	NE	ARG	394	21.282	-1.561	30.417	1.00	33.97
ATOM	701	CZ	ARG	394	21.864	-1.350	29.239	1.00	31.61
ATOM	702	NH1	ARG	394	21.208	-0.715	28.281	1.00	32.42
ATOM	703	NH2	ARG	394	23.098	-1.784	29.022	1.00	29.81
ATOM	704	C	ARG	394	18.911	1.697	34.180	1.00	36.69
ATOM	705	O	ARG	394	18.445	0.966	35.048	1.00	37.07
ATOM	706	N	SER	395	19.954	2.492	34.395	1.00	33.63
ATOM	707	CA	SER	395	20.603	2.564	35.701	1.00	35.69

	ATOM	708	CB	SER	395	22.112	2.784	35.540	1.00	32.94
	ATOM	709	OG	SER	395	22.696	1.811	34.688	1.00	32.37
	ATOM	710	C	SER	395	20.010	3.713	36.531	1.00	36.44
	ATOM	711	O	SER	395	20.389	3.916	37.687	1.00	38.68
	ATOM	712	N	MET	396	19.076	4.449	35.937	1.00	36.46
	ATOM	713	CA	MET	396	18.431	5.588	36.589	1.00	43.08
	ATOM	714	CB	MET	396	17.275	6.104	35.725	1.00	43.87
	ATOM	715	CG	MET	396	17.481	7.507	35.176	1.00	46.18
	ATOM	716	SD	MET	396	15.962	8.278	34.581	1.00	49.58
	ATOM	717	CE	MET	396	14.988	8.298	36.065	1.00	53.58
	ATOM	718	C	MET	396	17.906	5.303	37.992	1.00	46.18
	ATOM	719	O	MET	396	18.125	6.089	38.913	1.00	46.34
	ATOM	720	N	GLU	397	17.215	4.180	38.152	1.00	49.39
	ATOM	721	CA	GLU	397	16.645	3.821	39.444	1.00	52.12
	ATOM	722	CB	GLU	397	15.296	3.130	39.246	1.00	55.34
	ATOM	723	CG	GLU	397	14.166	4.073	38.873	1.00	58.86
	ATOM	724	CD	GLU	397	13.195	3.448	37.891	1.00	63.28
	ATOM	725	OE1	GLU	397	13.660	2.925	36.854	1.00	64.68
	ATOM	726	OE2	GLU	397	11.972	3.475	38.155	1.00	65.39
	ATOM	727	C	GLU	397	17.548	2.933	40.283	1.00	52.75
	ATOM	728	O	GLU	397	17.071	2.187	41.139	1.00	53.96
	ATOM	729	N	HIS	398	18.851	3.014	40.040	1.00	50.25
	ATOM	730	CA	HIS	398	19.813	2.220	40.792	1.00	49.34
	ATOM	731	CB	HIS	398	20.271	1.018	39.963	1.00	52.04
	ATOM	732	CG	HIS	398	19.187	0.017	39.721	1.00	53.95
	ATOM	733	CD2	HIS	398	18.750	-1.022	40.472	1.00	53.92
	ATOM	734	ND1	HIS	398	18.374	0.054	38.608	1.00	55.91
	ATOM	735	CE1	HIS	398	17.482	-0.917	38.685	1.00	55.53
	ATOM	736	NE2	HIS	398	17.688	-1.585	39.806	1.00	55.81
	ATOM	737	C	HIS	398	20.999	3.084	41.196	1.00	47.44
	ATOM	738	O	HIS	398	22.121	2.887	40.730	1.00	44.91
	ATOM	739	N	PRO	399	20.755	4.049	42.096	1.00	46.45
	ATOM	740	CD	PRO	399	19.443	4.300	42.721	1.00	47.27
	ATOM	741	CA	PRO	399	21.785	4.968	42.586	1.00	45.35
	ATOM	742	CB	PRO	399	21.127	5.631	43.793	1.00	47.40
	ATOM	743	CG	PRO	399	19.660	5.561	43.504	1.00	47.72
	ATOM	744	C	PRO	399	23.086	4.270	42.958	1.00	44.70
	ATOM	745	O	PRO	399	23.078	3.233	43.627	1.00	46.46
	ATOM	746	N	GLY	400	24.202	4.840	42.509	1.00	41.57
	ATOM	747	CA	GLY	400	25.506	4.281	42.813	1.00	39.84
	ATOM	748	C	GLY	400	25.907	3.047	42.022	1.00	37.85
	ATOM	749	O	GLY	400	27.027	2.560	42.176	1.00	40.48
	ATOM	750	N	LYS	401	25.012	2.537	41.180	1.00	36.39
	ATOM	751	CA	LYS	401	25.315	1.344	40.390	1.00	34.47
	ATOM	752	CB	LYS	401	24.562	0.130	40.947	1.00	36.12
	ATOM	753	CG	LYS	401	24.633	-0.007	42.466	1.00	39.30
	ATOM	754	CD	LYS	401	24.288	-1.429	42.903	1.00	44.38
	ATOM	755	CE	LYS	401	24.459	-1.605	44.408	1.00	46.68

	ATOM	756	NZ	LYS	401	24.968	-2.969	44.747	1.00	53.37
	ATOM	757	C	LYS	401	24.969	1.485	38.911	1.00	32.34
	ATOM	758	O	LYS	401	24.141	2.308	38.531	1.00	31.16
	ATOM	759	N	LEU	402	25.612	0.663	38.086	1.00	28.52
5	ATOM	760	CA	LEU	402	25.358	0.658	36.648	1.00	29.06
	ATOM	761	CB	LEU	402	26.661	0.847	35.867	1.00	29.26
	ATOM	762	CG	LEU	402	27.278	2.242	36.029	1.00	24.67
	ATOM	763	CD1	LEU	402	28.623	2.310	35.310	1.00	27.47
	ATOM	764	CD2	LEU	402	26.312	3.277	35.482	1.00	24.93
10	ATOM	765	C	LEU	402	24.755	-0.686	36.292	1.00	30.43
	ATOM	766	O	LEU	402	25.367	-1.727	36.535	1.00	31.36
	ATOM	767	N	LEU	403	23.552	-0.658	35.735	1.00	31.07
	ATOM	768	CA	LEU	403	22.873	-1.880	35.335	1.00	32.96
	ATOM	769	CB	LEU	403	21.361	-1.693	35.434	1.00	33.86
15	ATOM	770	CG	LEU	403	20.551	-2.991	35.415	1.00	39.29
	ATOM	771	CD1	LEU	403	20.584	-3.637	36.806	1.00	43.62
	ATOM	772	CD2	LEU	403	19.128	-2.689	34.998	1.00	41.32
	ATOM	773	C	LEU	403	23.255	-2.218	33.899	1.00	30.06
	ATOM	774	O	LEU	403	22.543	-1.870	32.956	1.00	31.63
20	ATOM	775	N	PHE	404	24.383	-2.893	33.733	1.00	29.19
	ATOM	776	CA	PHE	404	24.834	-3.256	32.403	1.00	28.93
	ATOM	777	CB	PHE	404	26.201	-3.929	32.493	1.00	30.05
	ATOM	778	CG	PHE	404	27.305	-2.998	32.926	1.00	30.78
	ATOM	779	CD1	PHE	404	27.794	-3.033	34.228	1.00	32.91
25	ATOM	780	CD2	PHE	404	27.848	-2.078	32.030	1.00	32.75
	ATOM	781	CE1	PHE	404	28.816	-2.160	34.638	1.00	34.73
	ATOM	782	CE2	PHE	404	28.864	-1.205	32.423	1.00	30.68
	ATOM	783	CZ	PHE	404	29.350	-1.242	33.727	1.00	31.43
	ATOM	784	C	PHE	404	23.809	-4.181	31.756	1.00	30.80
30	ATOM	785	O	PHE	404	23.625	-4.175	30.538	1.00	28.09
	ATOM	786	N	ALA	405	23.138	-4.967	32.594	1.00	30.25
	ATOM	787	CA	ALA	405	22.104	-5.910	32.163	1.00	29.78
	ATOM	788	CB	ALA	405	22.745	-7.172	31.598	1.00	29.97
	ATOM	789	C	ALA	405	21.309	-6.237	33.429	1.00	31.95
35	ATOM	790	O	ALA	405	21.785	-5.995	34.535	1.00	32.36
	ATOM	791	N	PRO	406	20.088	-6.779	33.288	1.00	34.40
	ATOM	792	CD	PRO	406	19.356	-7.102	32.053	1.00	35.81
	ATOM	793	CA	PRO	406	19.303	-7.101	34.490	1.00	36.41
	ATOM	794	CB	PRO	406	17.985	-7.654	33.935	1.00	35.38
40	ATOM	795	CG	PRO	406	17.922	-7.153	32.519	1.00	36.49
	ATOM	796	C	PRO	406	19.997	-8.084	35.433	1.00	37.32
	ATOM	797	O	PRO	406	19.698	-8.112	36.626	1.00	38.34
	ATOM	798	N	ASN	407	20.924	-8.877	34.902	1.00	36.69
	ATOM	799	CA	ASN	407	21.652	-9.847	35.712	1.00	38.85
45	ATOM	800	CB	ASN	407	21.582	-11.243	35.083	1.00	39.69
	ATOM	801	CG	ASN	407	22.232	-11.306	33.711	1.00	44.10
	ATOM	802	OD1	ASN	407	22.345	-10.296	33.009	1.00	37.78
	ATOM	803	ND2	ASN	407	22.660	-12.503	33.319	1.00	45.74

	ATOM	804	C	ASN	407	23.100	-9.435	35.874	1.00	38.12
	ATOM	805	O	ASN	407	23.965	-10.256	36.178	1.00	39.81
	ATOM	806	N	LEU	408	23.364	-8.149	35.671	1.00	37.80
	ATOM	807	CA	LEU	408	24.713	-7.631	35.799	1.00	36.89
	ATOM	808	CB	LEU	408	25.449	-7.720	34.459	1.00	36.09
	ATOM	809	CG	LEU	408	26.972	-7.609	34.550	1.00	35.08
	ATOM	810	CD1	LEU	408	27.525	-8.775	35.354	1.00	39.15
	ATOM	811	CD2	LEU	408	27.578	-7.587	33.158	1.00	36.85
	ATOM	812	C	LEU	408	24.670	-6.187	36.286	1.00	40.55
	ATOM	813	O	LEU	408	24.646	-5.248	35.491	1.00	38.29
	ATOM	814	N	LEU	409	24.644	-6.034	37.607	1.00	39.50
	ATOM	815	CA	LEU	409	24.606	-4.733	38.257	1.00	41.00
	ATOM	816	CB	LEU	409	23.392	-4.658	39.184	1.00	43.69
	ATOM	817	CG	LEU	409	23.164	-3.382	39.993	1.00	47.35
	ATOM	818	CD1	LEU	409	22.848	-2.233	39.058	1.00	47.09
	ATOM	819	CD2	LEU	409	22.014	-3.603	40.976	1.00	49.38
	ATOM	820	C	LEU	409	25.894	-4.566	39.060	1.00	41.80
	ATOM	821	O	LEU	409	26.178	-5.358	39.960	1.00	41.00
	ATOM	822	N	LEU	410	26.676	-3.544	38.727	1.00	39.23
	ATOM	823	CA	LEU	410	27.931	-3.296	39.423	1.00	40.45
	ATOM	824	CB	LEU	410	29.106	-3.354	38.442	1.00	41.59
	ATOM	825	CG	LEU	410	29.457	-4.660	37.716	1.00	44.87
	ATOM	826	CD1	LEU	410	30.972	-4.728	37.554	1.00	45.41
	ATOM	827	CD2	LEU	410	28.949	-5.872	38.484	1.00	47.02
	ATOM	828	C	LEU	410	27.946	-1.944	40.132	1.00	40.67
	ATOM	829	O	LEU	410	27.361	-0.970	39.652	1.00	40.22
	ATOM	830	N	ASP	411	28.610	-1.890	41.281	1.00	41.57
	ATOM	831	CA	ASP	411	28.717	-0.640	42.025	1.00	42.69
	ATOM	832	CB	ASP	411	28.490	-0.874	43.528	1.00	44.44
	ATOM	833	CG	ASP	411	29.655	-1.578	44.210	1.00	46.70
	ATOM	834	OD1	ASP	411	29.537	-1.849	45.426	1.00	51.44
	ATOM	835	OD2	ASP	411	30.680	-1.861	43.553	1.00	48.79
	ATOM	836	C	ASP	411	30.088	-0.016	41.779	1.00	43.70
	ATOM	837	O	ASP	411	30.933	-0.610	41.107	1.00	38.48
	ATOM	838	N	ARG	412	30.295	1.181	42.321	1.00	46.78
	ATOM	839	CA	ARG	412	31.554	1.905	42.171	1.00	49.97
	ATOM	840	CB	ARG	412	31.601	3.090	43.138	1.00	51.28
	ATOM	841	CG	ARG	412	30.971	4.364	42.614	1.00	54.77
	ATOM	842	CD	ARG	412	31.644	5.580	43.219	1.00	54.61
	ATOM	843	NE	ARG	412	33.071	5.615	42.912	1.00	56.53
	ATOM	844	CZ	ARG	412	33.827	6.708	42.985	1.00	61.90
	ATOM	845	NH1	ARG	412	33.291	7.866	43.356	1.00	63.48
	ATOM	846	NH2	ARG	412	35.120	6.645	42.682	1.00	61.21
	ATOM	847	C	ARG	412	32.771	1.026	42.429	1.00	50.29
	ATOM	848	O	ARG	412	33.628	0.866	41.561	1.00	51.02
	ATOM	849	N	ASN	413	32.844	0.469	43.633	1.00	51.94
	ATOM	850	CA	ASN	413	33.969	-0.375	44.021	1.00	53.15
	ATOM	851	CB	ASN	413	33.719	-0.980	45.403	1.00	55.88

	ATOM	852	CG	ASN	413	33.654	0.073	46.496	1.00	57.99
	ATOM	853	OD1	ASN	413	33.697	1.276	46.223	1.00	58.27
	ATOM	854	ND2	ASN	413	33.551	-0.375	47.742	1.00	57.90
	ATOM	855	C	ASN	413	34.235	-1.480	43.013	1.00	53.95
5	ATOM	856	O	ASN	413	35.386	-1.743	42.659	1.00	53.67
	ATOM	857	N	GLN	414	33.173	-2.129	42.547	1.00	55.33
	ATOM	858	CA	GLN	414	33.326	-3.198	41.573	1.00	55.42
	ATOM	859	CB	GLN	414	31.991	-3.904	41.343	1.00	55.44
	ATOM	860	CG	GLN	414	31.645	-4.933	42.391	1.00	56.07
10	ATOM	861	CD	GLN	414	30.203	-5.376	42.336	1.00	57.40
	ATOM	862	OE1	GLN	414	29.296	-4.536	42.402	1.00	60.22
	ATOM	863	NE2	GLN	414	29.973	-6.664	42.199	1.00	57.27
	ATOM	864	C	GLN	414	33.850	-2.630	40.259	1.00	55.51
	ATOM	865	O	GLN	414	34.654	-3.265	39.578	1.00	56.16
15	ATOM	866	N	GLY	415	33.398	-1.430	39.910	1.00	57.07
	ATOM	867	CA	GLY	415	33.849	-0.806	38.680	1.00	58.51
	ATOM	868	C	GLY	415	35.350	-0.582	38.689	1.00	61.10
	ATOM	869	O	GLY	415	36.023	-0.748	37.671	1.00	59.47
	ATOM	870	N	LYS	416	35.877	-0.211	39.851	1.00	62.77
20	ATOM	871	CA	LYS	416	37.305	0.041	40.011	1.00	65.49
	ATOM	872	CB	LYS	416	37.634	0.262	41.491	1.00	66.04
	ATOM	873	CG	LYS	416	38.121	1.663	41.823	1.00	68.71
	ATOM	874	CD	LYS	416	37.078	2.439	42.613	1.00	70.98
	ATOM	875	CE	LYS	416	37.404	2.448	44.100	1.00	71.84
25	ATOM	876	NZ	LYS	416	36.225	2.079	44.933	1.00	71.95
	ATOM	877	C	LYS	416	38.159	-1.105	39.472	1.00	66.41
	ATOM	878	O	LYS	416	39.361	-0.946	39.269	1.00	67.15
	ATOM	879	N	CYS	417	37.538	-2.257	39.238	1.00	67.33
	ATOM	880	CA	CYS	417	38.270	-3.414	38.741	1.00	68.16
30	ATOM	881	CB	CYS	417	37.951	-4.642	39.602	1.00	70.88
	ATOM	882	SG	CYS	417	38.592	-4.549	41.301	1.00	76.09
	ATOM	883	C	CYS	417	38.015	-3.736	37.270	1.00	67.54
	ATOM	884	O	CYS	417	38.632	-4.653	36.720	1.00	68.48
	ATOM	885	N	VAL	418	37.111	-2.994	36.631	1.00	64.67
35	ATOM	886	CA	VAL	418	36.817	-3.226	35.218	1.00	59.97
	ATOM	887	CB	VAL	418	35.326	-2.917	34.879	1.00	59.60
	ATOM	888	CG1	VAL	418	34.971	-1.503	35.284	1.00	59.13
	ATOM	889	CG2	VAL	418	35.072	-3.121	33.391	1.00	54.85
	ATOM	890	C	VAL	418	37.739	-2.362	34.355	1.00	58.37
40	ATOM	891	O	VAL	418	37.799	-1.140	34.512	1.00	55.44
	ATOM	892	N	GLU	419	38.463	-3.012	33.450	1.00	56.02
	ATOM	893	CA	GLU	419	39.403	-2.328	32.570	1.00	54.28
	ATOM	894	CB	GLU	419	40.149	-3.351	31.710	1.00	57.57
	ATOM	895	CG	GLU	419	39.385	-3.779	30.468	1.00	60.87
45	ATOM	896	CD	GLU	419	40.179	-4.722	29.584	1.00	63.34
	ATOM	897	OE1	GLU	419	40.432	-5.870	30.011	1.00	64.90
	ATOM	898	OE2	GLU	419	40.546	-4.313	28.462	1.00	63.18
	ATOM	899	C	GLU	419	38.761	-1.281	31.662	1.00	52.05

	ATOM	900	O	GLU	419	37.665	-1.481	31.131	1.00	49.82
	ATOM	901	N	GLY	420	39.465	-0.165	31.491	1.00	49.45
	ATOM	902	CA	GLY	420	38.983	0.908	30.642	1.00	46.22
	ATOM	903	C	GLY	420	37.895	1.767	31.254	1.00	44.55
5	ATOM	904	O	GLY	420	37.417	2.705	30.619	1.00	42.08
	ATOM	905	N	MET	421	37.503	1.471	32.488	1.00	43.41
	ATOM	906	CA	MET	421	36.449	2.248	33.123	1.00	42.48
	ATOM	907	CB	MET	421	35.306	1.327	33.554	1.00	42.34
	ATOM	908	CG	MET	421	34.590	0.635	32.396	1.00	38.22
10	ATOM	909	SD	MET	421	32.927	0.102	32.843	1.00	38.56
	ATOM	910	CE	MET	421	32.003	1.699	32.766	1.00	35.54
	ATOM	911	C	MET	421	36.923	3.059	34.312	1.00	41.64
	ATOM	912	O	MET	421	36.113	3.512	35.111	1.00	39.77
	ATOM	913	N	VAL	422	38.232	3.256	34.430	1.00	43.42
15	ATOM	914	CA	VAL	422	38.757	4.019	35.557	1.00	44.79
	ATOM	915	CB	VAL	422	40.285	4.248	35.433	1.00	46.54
	ATOM	916	CG1	VAL	422	40.595	5.086	34.206	1.00	48.25
	ATOM	917	CG2	VAL	422	40.813	4.920	36.696	1.00	46.24
	ATOM	918	C	VAL	422	38.056	5.372	35.689	1.00	44.09
20	ATOM	919	O	VAL	422	37.691	5.783	36.783	1.00	44.12
	ATOM	920	N	GLU	423	37.846	6.055	34.570	1.00	42.07
	ATOM	921	CA	GLU	423	37.192	7.356	34.616	1.00	40.24
	ATOM	922	CB	GLU	423	37.909	8.338	33.684	1.00	44.02
	ATOM	923	CG	GLU	423	39.411	8.467	33.893	1.00	50.04
25	ATOM	924	CD	GLU	423	40.096	9.158	32.719	1.00	55.64
	ATOM	925	OE1	GLU	423	39.539	10.156	32.205	1.00	56.66
	ATOM	926	OE2	GLU	423	41.188	8.703	32.306	1.00	58.02
	ATOM	927	C	GLU	423	35.704	7.337	34.250	1.00	35.77
	ATOM	928	O	GLU	423	34.881	7.955	34.919	1.00	33.20
30	ATOM	929	N	ILE	424	35.345	6.617	33.197	1.00	36.16
	ATOM	930	CA	ILE	424	33.949	6.643	32.771	1.00	31.63
	ATOM	931	CB	ILE	424	33.803	6.087	31.347	1.00	33.58
	ATOM	932	CG2	ILE	424	34.639	6.936	30.395	1.00	33.48
	ATOM	933	CG1	ILE	424	34.204	4.617	31.296	1.00	34.46
35	ATOM	934	CD1	ILE	424	33.857	3.955	29.978	1.00	34.67
	ATOM	935	C	ILE	424	32.890	6.035	33.685	1.00	28.89
	ATOM	936	O	ILE	424	31.729	6.443	33.632	1.00	26.49
	ATOM	937	N	PHE	425	33.261	5.091	34.542	1.00	29.26
	ATOM	938	CA	PHE	425	32.257	4.520	35.447	1.00	29.87
40	ATOM	939	CB	PHE	425	32.903	3.529	36.423	1.00	31.26
	ATOM	940	CG	PHE	425	31.948	2.496	36.959	1.00	32.17
	ATOM	941	CD1	PHE	425	31.124	2.783	38.048	1.00	33.70
	ATOM	942	CD2	PHE	425	31.881	1.230	36.381	1.00	30.64
	ATOM	943	CE1	PHE	425	30.244	1.814	38.563	1.00	32.60
45	ATOM	944	CE2	PHE	425	31.010	0.256	36.881	1.00	31.55
	ATOM	945	CZ	PHE	425	30.189	0.549	37.973	1.00	33.34
	ATOM	946	C	PHE	425	31.594	5.649	36.240	1.00	30.17
	ATOM	947	O	PHE	425	30.368	5.774	36.276	1.00	26.71

	ATOM	948	N	ASP	426	32.415	6.483	36.870	1.00	29.45
	ATOM	949	CA	ASP	426	31.893	7.587	37.661	1.00	32.29
	ATOM	950	CB	ASP	426	33.031	8.291	38.401	1.00	33.49
	ATOM	951	CG	ASP	426	33.455	7.546	39.655	1.00	39.42
5	ATOM	952	OD1	ASP	426	32.767	6.574	40.038	1.00	38.35
	ATOM	953	OD2	ASP	426	34.480	7.934	40.256	1.00	39.58
	ATOM	954	C	ASP	426	31.133	8.592	36.806	1.00	29.02
	ATOM	955	O	ASP	426	30.154	9.175	37.257	1.00	31.34
	ATOM	956	N	MET	427	31.585	8.797	35.572	1.00	30.69
10	ATOM	957	CA	MET	427	30.919	9.736	34.675	1.00	28.63
	ATOM	958	CB	MET	427	31.744	9.912	33.407	1.00	26.83
	ATOM	959	CG	MET	427	33.032	10.680	33.608	1.00	31.41
	ATOM	960	SD	MET	427	33.962	10.783	32.077	1.00	34.87
	ATOM	961	CE	MET	427	35.409	11.753	32.643	1.00	44.60
15	ATOM	962	C	MET	427	29.526	9.202	34.324	1.00	28.70
	ATOM	963	O	MET	427	28.536	9.947	34.302	1.00	25.01
	ATOM	964	N	LEU	428	29.451	7.902	34.057	1.00	25.13
	ATOM	965	CA	LEU	428	28.173	7.292	33.730	1.00	27.60
	ATOM	966	CB	LEU	428	28.379	5.824	33.332	1.00	28.00
20	ATOM	967	CG	LEU	428	29.039	5.682	31.957	1.00	26.99
	ATOM	968	CD1	LEU	428	29.678	4.303	31.782	1.00	27.80
	ATOM	969	CD2	LEU	428	27.995	5.927	30.894	1.00	25.33
	ATOM	970	C	LEU	428	27.210	7.412	34.916	1.00	29.59
	ATOM	971	O	LEU	428	26.041	7.743	34.743	1.00	27.07
25	ATOM	972	N	LEU	429	27.701	7.147	36.126	1.00	30.40
	ATOM	973	CA	LEU	429	26.859	7.251	37.323	1.00	30.59
	ATOM	974	CB	LEU	429	27.675	6.884	38.571	1.00	31.76
	ATOM	975	CG	LEU	429	28.078	5.415	38.757	1.00	32.43
	ATOM	976	CD1	LEU	429	28.961	5.264	39.995	1.00	31.60
30	ATOM	977	CD2	LEU	429	26.825	4.573	38.903	1.00	34.66
	ATOM	978	C	LEU	429	26.319	8.681	37.466	1.00	30.46
	ATOM	979	O	LEU	429	25.143	8.901	37.769	1.00	28.40
	ATOM	980	N	ALA	430	27.193	9.656	37.237	1.00	31.34
	ATOM	981	CA	ALA	430	26.806	11.059	37.332	1.00	29.83
35	ATOM	982	CB	ALA	430	28.017	11.951	37.078	1.00	31.29
	ATOM	983	C	ALA	430	25.696	11.387	36.344	1.00	31.04
	ATOM	984	O	ALA	430	24.753	12.107	36.674	1.00	30.79
	ATOM	985	N	THR	431	25.802	10.854	35.128	1.00	30.30
	ATOM	986	CA	THR	431	24.786	11.105	34.112	1.00	28.81
40	ATOM	987	CB	THR	431	25.207	10.533	32.737	1.00	30.55
	ATOM	988	OG1	THR	431	26.569	10.893	32.465	1.00	31.88
	ATOM	989	CG2	THR	431	24.321	11.087	31.634	1.00	25.63
	ATOM	990	C	THR	431	23.462	10.481	34.530	1.00	29.49
	ATOM	991	O	THR	431	22.402	11.099	34.397	1.00	26.18
45	ATOM	992	N	SER	432	23.520	9.253	35.037	1.00	28.11
	ATOM	993	CA	SER	432	22.308	8.573	35.480	1.00	29.78
	ATOM	994	CB	SER	432	22.639	7.177	36.008	1.00	33.11
	ATOM	995	OG	SER	432	21.454	6.412	36.136	1.00	36.92

	ATOM	996	C	SER	432	21.651	9.399	36.589	1.00	31.49
	ATOM	997	O	SER	432	20.433	9.576	36.613	1.00	30.09
	ATOM	998	N	ASER	433	22.476	9.901	37.496	0.75	32.09
	ATOM	999	N	BSER	433	22.474	9.906	37.500	0.25	31.10
	ATOM	1000	CA	ASER	433	22.002	10.715	38.605	0.75	35.68
	ATOM	1001	CA	BSER	433	21.985	10.717	38.608	0.25	32.21
	ATOM	1002	CB	ASER	433	23.185	11.097	39.502	0.75	37.18
	ATOM	1003	CB	BSER	433	23.145	11.104	39.529	0.25	31.45
	ATOM	1004	OG	ASER	433	22.823	12.090	40.443	0.75	44.09
	ATOM	1005	OG	BSER	433	23.785	9.953	40.053	0.25	29.52
	ATOM	1006	C	ASER	433	21.299	11.971	38.091	0.75	35.01
	ATOM	1007	C	BSER	433	21.295	11.976	38.092	0.25	32.88
	ATOM	1008	O	ASER	433	20.257	12.373	38.612	0.75	35.34
	ATOM	1009	O	BSER	433	20.264	12.391	38.622	0.25	33.42
	ATOM	1010	N	ARG	434	21.867	12.579	37.054	1.00	33.38
	ATOM	1011	CA	ARG	434	21.300	13.788	36.470	1.00	34.19
	ATOM	1012	CB	ARG	434	22.239	14.354	35.400	1.00	33.89
	ATOM	1013	CG	ARG	434	21.670	15.528	34.625	1.00	38.30
	ATOM	1014	CD	ARG	434	21.559	16.787	35.479	1.00	37.91
	ATOM	1015	NE	ARG	434	21.158	17.944	34.680	1.00	37.78
	ATOM	1016	CZ	ARG	434	20.488	18.995	35.149	1.00	41.06
	ATOM	1017	NH1	ARG	434	20.132	19.049	36.428	1.00	40.70
	ATOM	1018	NH2	ARG	434	20.175	19.998	34.337	1.00	38.78
	ATOM	1019	C	ARG	434	19.937	13.491	35.873	1.00	33.48
	ATOM	1020	O	ARG	434	18.996	14.266	36.053	1.00	30.54
	ATOM	1021	N	PHE	435	19.831	12.371	35.158	1.00	34.68
	ATOM	1022	CA	PHE	435	18.563	11.963	34.549	1.00	35.02
	ATOM	1023	CB	PHE	435	18.727	10.634	33.796	1.00	34.96
	ATOM	1024	CG	PHE	435	19.240	10.779	32.386	1.00	37.63
	ATOM	1025	CD1	PHE	435	19.459	12.035	31.824	1.00	42.03
	ATOM	1026	CD2	PHE	435	19.521	9.649	31.623	1.00	41.24
	ATOM	1027	CE1	PHE	435	19.953	12.164	30.521	1.00	43.11
	ATOM	1028	CE2	PHE	435	20.016	9.768	30.322	1.00	40.59
	ATOM	1029	CZ	PHE	435	20.233	11.029	29.775	1.00	40.63
	ATOM	1030	C	PHE	435	17.527	11.780	35.657	1.00	35.49
	ATOM	1031	O	PHE	435	16.361	12.135	35.496	1.00	34.78
	ATOM	1032	N	ARG	436	17.968	11.216	36.777	1.00	38.27
	ATOM	1033	CA	ARG	436	17.094	10.982	37.924	1.00	40.67
	ATOM	1034	CB	ARG	436	17.844	10.215	39.012	1.00	40.70
	ATOM	1035	CG	ARG	436	16.942	9.590	40.068	1.00	44.98
	ATOM	1036	CD	ARG	436	17.648	8.459	40.810	1.00	48.09
	ATOM	1037	NE	ARG	436	18.982	8.841	41.275	1.00	50.16
	ATOM	1038	CZ	ARG	436	20.119	8.361	40.777	1.00	52.19
	ATOM	1039	NH1	ARG	436	20.099	7.472	39.790	1.00	49.34
	ATOM	1040	NH2	ARG	436	21.283	8.770	41.266	1.00	51.85
	ATOM	1041	C	ARG	436	16.576	12.302	38.493	1.00	40.40
	ATOM	1042	O	ARG	436	15.382	12.458	38.730	1.00	41.49
	ATOM	1043	N	MET	437	17.477	13.252	38.706	1.00	40.02

	ATOM	1044	CA	MET	437	17.090	14.546	39.245	1.00	41.02
	ATOM	1045	CB	MET	437	18.329	15.427	39.440	1.00	40.29
	ATOM	1046	C	MET	437	16.099	15.221	38.299	1.00	40.81
	ATOM	1047	O	MET	437	15.111	15.805	38.734	1.00	42.46
5	ATOM	1048	N	MET	438	16.367	15.127	37.001	1.00	39.02
	ATOM	1049	CA	MET	438	15.510	15.732	35.988	1.00	40.11
	ATOM	1050	CB	MET	438	16.237	15.793	34.651	1.00	38.16
	ATOM	1051	CG	MET	438	17.352	16.794	34.601	1.00	41.52
	ATOM	1052	SD	MET	438	17.999	16.862	32.943	1.00	43.94
10	ATOM	1053	CE	MET	438	16.698	17.748	32.096	1.00	39.96
	ATOM	1054	C	MET	438	14.221	14.964	35.783	1.00	37.72
	ATOM	1055	O	MET	438	13.305	15.451	35.125	1.00	36.82
	ATOM	1056	N	ASN	439	14.155	13.759	36.337	1.00	38.81
	ATOM	1057	CA	ASN	439	12.981	12.919	36.174	1.00	40.77
15	ATOM	1058	CB	ASN	439	11.762	13.556	36.847	1.00	44.52
	ATOM	1059	CG	ASN	439	10.566	12.620	36.887	1.00	48.29
	ATOM	1060	OD1	ASN	439	10.721	11.400	36.964	1.00	48.48
	ATOM	1061	ND2	ASN	439	9.365	13.189	36.829	1.00	50.23
	ATOM	1062	C	ASN	439	12.725	12.744	34.677	1.00	39.36
20	ATOM	1063	O	ASN	439	11.637	13.037	34.172	1.00	37.76
	ATOM	1064	N	LEU	440	13.749	12.274	33.972	1.00	37.65
	ATOM	1065	CA	LEU	440	13.655	12.052	32.532	1.00	35.22
	ATOM	1066	CB	LEU	440	14.999	11.576	31.987	1.00	34.70
	ATOM	1067	CG	LEU	440	15.022	11.467	30.462	1.00	35.45
25	ATOM	1068	CD1	LEU	440	14.890	12.862	29.869	1.00	35.24
	ATOM	1069	CD2	LEU	440	16.297	10.795	29.999	1.00	35.30
	ATOM	1070	C	LEU	440	12.587	11.024	32.196	1.00	36.48
	ATOM	1071	O	LEU	440	12.518	9.967	32.826	1.00	37.36
	ATOM	1072	N	GLN	441	11.763	11.328	31.197	1.00	36.82
30	ATOM	1073	CA	GLN	441	10.696	10.420	30.785	1.00	38.51
	ATOM	1074	CB	GLN	441	9.431	11.211	30.443	1.00	38.23
	ATOM	1075	CG	GLN	441	8.912	12.063	31.592	1.00	42.46
	ATOM	1076	CD	GLN	441	8.362	11.227	32.729	1.00	44.91
	ATOM	1077	OE1	GLN	441	7.268	10.668	32.629	1.00	47.31
35	ATOM	1078	NE2	GLN	441	9.119	11.132	33.818	1.00	44.06
	ATOM	1079	C	GLN	441	11.099	9.565	29.585	1.00	38.48
	ATOM	1080	O	GLN	441	11.923	9.976	28.763	1.00	35.80
	ATOM	1081	N	GLY	442	10.500	8.378	29.494	1.00	36.03
	ATOM	1082	CA	GLY	442	10.792	7.468	28.401	1.00	37.72
40	ATOM	1083	C	GLY	442	10.599	8.112	27.043	1.00	36.88
	ATOM	1084	O	GLY	442	11.381	7.877	26.123	1.00	33.72
	ATOM	1085	N	GLU	443	9.556	8.925	26.918	1.00	36.59
	ATOM	1086	CA	GLU	443	9.269	9.603	25.661	1.00	37.13
	ATOM	1087	CB	GLU	443	7.956	10.379	25.764	1.00	41.57
45	ATOM	1088	CG	GLU	443	6.723	9.488	25.879	1.00	47.76
	ATOM	1089	CD	GLU	443	6.483	9.008	27.302	1.00	53.96
	ATOM	1090	OE1	GLU	443	5.619	8.123	27.498	1.00	57.66
	ATOM	1091	OE2	GLU	443	7.159	9.515	28.225	1.00	56.13

	ATOM	1092	C	GLU	443	10.408	10.551	25.311	1.00	35.27
	ATOM	1093	O	GLU	443	10.759	10.704	24.145	1.00	33.85
	ATOM	1094	N	GLU	444	10.984	11.179	26.331	1.00	32.09
	ATOM	1095	CA	GLU	444	12.097	12.095	26.126	1.00	33.92
5	ATOM	1096	CB	GLU	444	12.332	12.924	27.388	1.00	34.97
	ATOM	1097	CG	GLU	444	11.169	13.845	27.732	1.00	38.28
	ATOM	1098	CD	GLU	444	11.383	14.610	29.023	1.00	38.11
	ATOM	1099	OE1	GLU	444	11.800	13.993	30.026	1.00	39.53
	ATOM	1100	OE2	GLU	444	11.132	15.834	29.036	1.00	40.77
10	ATOM	1101	C	GLU	444	13.356	11.305	25.770	1.00	33.59
	ATOM	1102	O	GLU	444	14.085	11.670	24.842	1.00	33.35
	ATOM	1103	N	PHE	445	13.590	10.215	26.501	1.00	30.68
	ATOM	1104	CA	PHE	445	14.753	9.357	26.276	1.00	32.49
	ATOM	1105	CB	PHE	445	14.703	8.139	27.203	1.00	29.35
15	ATOM	1106	CG	PHE	445	15.667	7.047	26.828	1.00	30.78
	ATOM	1107	CD1	PHE	445	17.036	7.201	27.030	1.00	28.25
	ATOM	1108	CD2	PHE	445	15.205	5.863	26.266	1.00	30.62
	ATOM	1109	CE1	PHE	445	17.933	6.195	26.675	1.00	28.67
	ATOM	1110	CE2	PHE	445	16.095	4.848	25.908	1.00	31.37
20	ATOM	1111	CZ	PHE	445	17.460	5.015	26.113	1.00	30.37
	ATOM	1112	C	PHE	445	14.850	8.885	24.829	1.00	31.11
	ATOM	1113	O	PHE	445	15.924	8.947	24.221	1.00	32.20
	ATOM	1114	N	VAL	446	13.739	8.415	24.266	1.00	28.63
	ATOM	1115	CA	VAL	446	13.787	7.943	22.889	1.00	27.94
25	ATOM	1116	CB	VAL	446	12.478	7.193	22.478	1.00	28.48
	ATOM	1117	CG1	VAL	446	12.318	5.939	23.343	1.00	29.61
	ATOM	1118	CG2	VAL	446	11.265	8.092	22.607	1.00	27.23
	ATOM	1119	C	VAL	446	14.099	9.064	21.900	1.00	27.28
	ATOM	1120	O	VAL	446	14.781	8.837	20.904	1.00	28.07
30	ATOM	1121	N	CYS	447	13.619	10.275	22.166	1.00	28.97
	ATOM	1122	CA	CYS	447	13.919	11.394	21.272	1.00	29.14
	ATOM	1123	CB	CYS	447	13.156	12.653	21.693	1.00	28.90
	ATOM	1124	SG	CYS	447	11.389	12.591	21.309	1.00	35.68
	ATOM	1125	C	CYS	447	15.420	11.677	21.328	1.00	28.03
35	ATOM	1126	O	CYS	447	16.063	11.885	20.302	1.00	29.34
	ATOM	1127	N	LEU	448	15.969	11.686	22.538	1.00	27.28
	ATOM	1128	CA	LEU	448	17.392	11.938	22.729	1.00	25.30
	ATOM	1129	CB	LEU	448	17.733	11.932	24.220	1.00	27.72
	ATOM	1130	CG	LEU	448	17.248	13.135	25.040	1.00	29.54
40	ATOM	1131	CD1	LEU	448	17.807	13.042	26.454	1.00	30.85
	ATOM	1132	CD2	LEU	448	17.688	14.434	24.376	1.00	30.24
	ATOM	1133	C	LEU	448	18.245	10.902	22.008	1.00	27.62
	ATOM	1134	O	LEU	448	19.207	11.252	21.327	1.00	25.10
	ATOM	1135	N	LYS	449	17.905	9.621	22.162	1.00	25.16
45	ATOM	1136	CA	LYS	449	18.673	8.570	21.506	1.00	27.55
	ATOM	1137	CB	LYS	449	18.135	7.185	21.900	1.00	28.99
	ATOM	1138	CG	LYS	449	19.134	6.052	21.694	1.00	34.70
	ATOM	1139	CD	LYS	449	18.737	4.789	22.459	1.00	32.67

	ATOM	1140	CE	LYS	449	17.267	4.419	22.220	1.00	31.87
	ATOM	1141	NZ	LYS	449	17.022	2.967	22.472	1.00	29.14
	ATOM	1142	C	LYS	449	18.626	8.749	19.990	1.00	25.88
	ATOM	1143	O	LYS	449	19.610	8.489	19.296	1.00	25.93
	ATOM	1144	N	SER	450	17.482	9.197	19.480	1.00	26.07
	ATOM	1145	CA	SER	450	17.323	9.421	18.052	1.00	27.24
	ATOM	1146	CB	SER	450	15.857	9.705	17.721	1.00	32.24
	ATOM	1147	OG	SER	450	15.098	8.519	17.779	1.00	34.94
	ATOM	1148	C	SER	450	18.176	10.607	17.618	1.00	26.78
	ATOM	1149	O	SER	450	18.763	10.598	16.535	1.00	25.85
	ATOM	1150	N	ILE	451	18.231	11.632	18.463	1.00	26.94
	ATOM	1151	CA	ILE	451	19.032	12.810	18.155	1.00	26.13
	ATOM	1152	CB	ILE	451	18.950	13.850	19.291	1.00	27.72
	ATOM	1153	CG2	ILE	451	20.019	14.929	19.101	1.00	20.53
	ATOM	1154	CG1	ILE	451	17.553	14.475	19.322	1.00	29.49
	ATOM	1155	CD1	ILE	451	17.377	15.473	20.447	1.00	36.24
	ATOM	1156	C	ILE	451	20.489	12.381	17.989	1.00	24.88
	ATOM	1157	O	ILE	451	21.161	12.771	17.034	1.00	26.96
	ATOM	1158	N	ILE	452	20.977	11.582	18.931	1.00	22.72
	ATOM	1159	CA	ILE	452	22.359	11.120	18.880	1.00	21.95
	ATOM	1160	CB	ILE	452	22.660	10.155	20.050	1.00	23.57
	ATOM	1161	CG2	ILE	452	23.982	9.435	19.804	1.00	22.10
	ATOM	1162	CG1	ILE	452	22.718	10.949	21.371	1.00	21.70
	ATOM	1163	CD1	ILE	452	22.768	10.060	22.624	1.00	25.30
	ATOM	1164	C	ILE	452	22.656	10.419	17.557	1.00	23.02
	ATOM	1165	O	ILE	452	23.650	10.708	16.885	1.00	21.25
	ATOM	1166	N	LEU	453	21.779	9.497	17.173	1.00	22.83
	ATOM	1167	CA	LEU	453	21.984	8.768	15.935	1.00	22.05
	ATOM	1168	CB	LEU	453	20.843	7.764	15.733	1.00	22.06
	ATOM	1169	CG	LEU	453	20.712	7.189	14.324	1.00	22.03
	ATOM	1170	CD1	LEU	453	21.815	6.165	14.107	1.00	24.81
	ATOM	1171	CD2	LEU	453	19.328	6.535	14.156	1.00	24.73
	ATOM	1172	C	LEU	453	22.092	9.687	14.717	1.00	23.95
	ATOM	1173	O	LEU	453	22.962	9.501	13.860	1.00	24.60
	ATOM	1174	N	LEU	454	21.220	10.687	14.638	1.00	26.72
	ATOM	1175	CA	LEU	454	21.234	11.599	13.494	1.00	26.45
	ATOM	1176	CB	LEU	454	19.852	12.242	13.330	1.00	25.51
	ATOM	1177	CG	LEU	454	18.737	11.222	13.052	1.00	30.16
	ATOM	1178	CD1	LEU	454	17.405	11.926	12.955	1.00	28.76
	ATOM	1179	CD2	LEU	454	19.037	10.478	11.759	1.00	32.59
	ATOM	1180	C	LEU	454	22.292	12.703	13.552	1.00	28.24
	ATOM	1181	O	LEU	454	22.778	13.148	12.513	1.00	29.06
	ATOM	1182	N	ASN	455	22.638	13.146	14.757	1.00	26.56
	ATOM	1183	CA	ASN	455	23.604	14.236	14.934	1.00	26.79
	ATOM	1184	CB	ASN	455	23.284	14.998	16.224	1.00	26.20
	ATOM	1185	CG	ASN	455	24.174	16.217	16.419	1.00	27.26
	ATOM	1186	OD1	ASN	455	24.171	17.134	15.602	1.00	30.83
	ATOM	1187	ND2	ASN	455	24.931	16.230	17.506	1.00	27.16

	ATOM	1188	C	ASN	455	25.062	13.782	14.954	1.00	30.63
	ATOM	1189	O	ASN	455	25.965	14.517	14.525	1.00	27.69
	ATOM	1190	N	SER	456	25.268	12.569	15.461	1.00	30.48
	ATOM	1191	CA	SER	456	26.572	11.928	15.579	1.00	35.26
5	ATOM	1192	CB	SER	456	26.393	10.393	15.505	1.00	39.69
	ATOM	1193	OG	SER	456	25.871	9.953	14.243	1.00	30.73
	ATOM	1194	C	SER	456	27.627	12.344	14.562	1.00	35.56
	ATOM	1195	O	SER	456	28.599	13.041	14.884	1.00	33.00
	ATOM	1196	N	GLY	457	27.437	11.886	13.334	1.00	33.88
10	ATOM	1197	CA	GLY	457	28.393	12.189	12.292	1.00	36.77
	ATOM	1198	C	GLY	457	27.876	13.017	11.136	1.00	37.02
	ATOM	1199	O	GLY	457	28.310	12.805	10.013	1.00	38.66
	ATOM	1200	N	VAL	458	26.967	13.956	11.392	1.00	39.12
	ATOM	1201	CA	VAL	458	26.438	14.802	10.317	1.00	43.81
15	ATOM	1202	CB	VAL	458	25.231	15.648	10.755	1.00	44.25
	ATOM	1203	CG1	VAL	458	24.209	15.713	9.631	1.00	44.51
	ATOM	1204	CG2	VAL	458	24.638	15.098	12.013	1.00	50.53
	ATOM	1205	C	VAL	458	27.472	15.801	9.817	1.00	46.72
	ATOM	1206	O	VAL	458	27.391	16.265	8.681	1.00	47.08
20	ATOM	1207	N	TYR	459	28.432	16.144	10.670	1.00	50.74
	ATOM	1208	CA	TYR	459	29.456	17.114	10.301	1.00	55.43
	ATOM	1209	CB	TYR	459	29.647	18.129	11.433	1.00	56.62
	ATOM	1210	CG	TYR	459	28.375	18.870	11.781	1.00	59.34
	ATOM	1211	CD1	TYR	459	28.094	19.229	13.095	1.00	60.73
25	ATOM	1212	CE1	TYR	459	26.900	19.867	13.429	1.00	62.14
	ATOM	1213	CD2	TYR	459	27.430	19.175	10.795	1.00	62.16
	ATOM	1214	CE2	TYR	459	26.234	19.812	11.118	1.00	63.83
	ATOM	1215	CZ	TYR	459	25.976	20.154	12.437	1.00	62.88
	ATOM	1216	OH	TYR	459	24.790	20.764	12.767	1.00	62.56
30	ATOM	1217	C	TYR	459	30.791	16.489	9.928	1.00	57.21
	ATOM	1218	O	TYR	459	31.793	17.189	9.798	1.00	56.86
	ATOM	1219	N	THR	460	30.800	15.173	9.750	1.00	59.22
	ATOM	1220	CA	THR	460	32.018	14.474	9.366	1.00	62.25
	ATOM	1221	CB	THR	460	32.502	13.531	10.499	1.00	63.07
35	ATOM	1222	OG1	THR	460	33.474	12.613	9.983	1.00	67.80
	ATOM	1223	CG2	THR	460	31.344	12.759	11.084	1.00	60.23
	ATOM	1224	C	THR	460	31.759	13.678	8.086	1.00	63.54
	ATOM	1225	O	THR	460	32.457	12.708	7.782	1.00	63.91
	ATOM	1226	N	PHE	461	30.758	14.113	7.326	1.00	65.06
40	ATOM	1227	CA	PHE	461	30.395	13.446	6.080	1.00	67.00
	ATOM	1228	CB	PHE	461	29.052	13.975	5.563	1.00	66.48
	ATOM	1229	CG	PHE	461	27.867	13.147	5.991	1.00	66.30
	ATOM	1230	CD1	PHE	461	26.657	13.754	6.312	1.00	65.58
	ATOM	1231	CD2	PHE	461	27.963	11.760	6.085	1.00	66.41
45	ATOM	1232	CE1	PHE	461	25.562	12.996	6.723	1.00	65.45
	ATOM	1233	CE2	PHE	461	26.872	10.994	6.494	1.00	66.83
	ATOM	1234	CZ	PHE	461	25.670	11.616	6.814	1.00	65.12
	ATOM	1235	C	PHE	461	31.463	13.604	5.004	1.00	68.38

ATOM	1236	O	PHE	461	32.181	14.606	4.962	1.00	68.98
ATOM	1237	N	LEU	462	31.542	12.601	4.132	1.00	69.57
ATOM	1238	CA	LEU	462	32.511	12.545	3.039	1.00	71.68
ATOM	1239	CB	LEU	462	32.080	11.475	2.030	1.00	71.00
ATOM	1240	C	LEU	462	32.810	13.856	2.304	1.00	72.40
ATOM	1241	O	LEU	462	33.725	14.590	2.680	1.00	73.45
ATOM	1242	N	SER	463	32.043	14.141	1.253	1.00	73.22
ATOM	1243	CA	SER	463	32.262	15.343	0.449	1.00	72.61
ATOM	1244	CB	SER	463	32.544	14.942	-1.005	1.00	73.38
ATOM	1245	C	SER	463	31.126	16.362	0.491	1.00	71.17
ATOM	1246	O	SER	463	30.455	16.528	1.511	1.00	72.05
ATOM	1247	N	SER	464	30.932	17.049	-0.633	1.00	68.86
ATOM	1248	CA	SER	464	29.892	18.063	-0.759	1.00	66.06
ATOM	1249	CB	SER	464	30.514	19.457	-0.704	1.00	66.26
ATOM	1250	C	SER	464	29.108	17.887	-2.060	1.00	63.72
ATOM	1251	O	SER	464	28.657	18.862	-2.662	1.00	62.88
ATOM	1252	N	THR	465	28.954	16.638	-2.493	1.00	60.93
ATOM	1253	CA	THR	465	28.205	16.343	-3.709	1.00	57.47
ATOM	1254	CB	THR	465	28.185	14.824	-4.004	1.00	57.80
ATOM	1255	OG1	THR	465	27.525	14.135	-2.934	1.00	54.75
ATOM	1256	CG2	THR	465	29.606	14.287	-4.149	1.00	57.49
ATOM	1257	C	THR	465	26.767	16.824	-3.523	1.00	54.93
ATOM	1258	O	THR	465	26.349	17.129	-2.407	1.00	54.26
ATOM	1259	N	LEU	466	26.013	16.892	-4.614	1.00	51.85
ATOM	1260	CA	LEU	466	24.625	17.330	-4.550	1.00	49.25
ATOM	1261	CB	LEU	466	24.013	17.349	-5.956	1.00	48.74
ATOM	1262	CG	LEU	466	22.953	18.415	-6.253	1.00	48.72
ATOM	1263	CD1	LEU	466	22.156	18.002	-7.482	1.00	48.32
ATOM	1264	CD2	LEU	466	22.033	18.594	-5.057	1.00	48.14
ATOM	1265	C	LEU	466	23.817	16.397	-3.650	1.00	48.16
ATOM	1266	O	LEU	466	22.961	16.845	-2.883	1.00	45.90
ATOM	1267	N	LYS	467	24.093	15.099	-3.750	1.00	46.47
ATOM	1268	CA	LYS	467	23.399	14.100	-2.947	1.00	47.45
ATOM	1269	CB	LYS	467	23.802	12.693	-3.395	1.00	49.38
ATOM	1270	CG	LYS	467	22.829	11.602	-2.974	1.00	52.70
ATOM	1271	CD	LYS	467	23.561	10.301	-2.682	1.00	56.48
ATOM	1272	CE	LYS	467	23.105	9.180	-3.604	1.00	59.54
ATOM	1273	NZ	LYS	467	24.150	8.117	-3.732	1.00	61.22
ATOM	1274	C	LYS	467	23.738	14.284	-1.472	1.00	46.89
ATOM	1275	O	LYS	467	22.884	14.108	-0.604	1.00	46.06
ATOM	1276	N	SER	468	24.989	14.644	-1.202	1.00	45.82
ATOM	1277	CA	SER	468	25.457	14.854	0.160	1.00	46.82
ATOM	1278	CB	SER	468	26.976	15.050	0.173	1.00	47.85
ATOM	1279	OG	SER	468	27.407	15.537	1.435	1.00	55.73
ATOM	1280	C	SER	468	24.778	16.063	0.790	1.00	44.24
ATOM	1281	O	SER	468	24.473	16.062	1.983	1.00	42.98
ATOM	1282	N	LEU	469	24.547	17.100	-0.011	1.00	42.33
ATOM	1283	CA	LEU	469	23.890	18.301	0.486	1.00	40.42

ATOM	1284	CB	LEU	469	24.002	19.427	-0.545	1.00	44.47
ATOM	1285	CG	LEU	469	25.438	19.874	-0.849	1.00	46.70
ATOM	1286	CD1	LEU	469	25.514	20.477	-2.246	1.00	46.70
ATOM	1287	CD2	LEU	469	25.890	20.883	0.199	1.00	47.32
ATOM	1288	C	LEU	469	22.423	17.996	0.786	1.00	39.06
ATOM	1289	O	LEU	469	21.856	18.505	1.760	1.00	34.97
ATOM	1290	N	GLU	470	21.814	17.151	-0.046	1.00	35.46
ATOM	1291	CA	GLU	470	20.418	16.768	0.145	1.00	34.38
ATOM	1292	CB	GLU	470	19.914	15.963	-1.052	1.00	38.02
ATOM	1293	CG	GLU	470	19.772	16.773	-2.329	1.00	42.67
ATOM	1294	CD	GLU	470	19.339	15.923	-3.509	1.00	48.30
ATOM	1295	OE1	GLU	470	19.671	14.716	-3.538	1.00	50.53
ATOM	1296	OE2	GLU	470	18.666	16.463	-4.412	1.00	51.06
ATOM	1297	C	GLU	470	20.290	15.916	1.403	1.00	34.37
ATOM	1298	O	GLU	470	19.321	16.035	2.157	1.00	32.60
ATOM	1299	N	GLU	471	21.274	15.046	1.606	1.00	34.66
ATOM	1300	CA	GLU	471	21.309	14.162	2.766	1.00	35.68
ATOM	1301	CB	GLU	471	22.515	13.222	2.671	1.00	34.57
ATOM	1302	CG	GLU	471	22.376	12.122	1.614	1.00	37.98
ATOM	1303	CD	GLU	471	21.476	10.989	2.063	1.00	39.79
ATOM	1304	OE1	GLU	471	20.268	11.027	1.743	1.00	41.12
ATOM	1305	OE2	GLU	471	21.974	10.061	2.737	1.00	32.11
ATOM	1306	C	GLU	471	21.393	14.983	4.052	1.00	34.79
ATOM	1307	O	GLU	471	20.596	14.793	4.969	1.00	32.80
ATOM	1308	N	LYS	472	22.358	15.898	4.112	1.00	33.93
ATOM	1309	CA	LYS	472	22.518	16.739	5.291	1.00	35.58
ATOM	1310	CB	LYS	472	23.683	17.710	5.097	1.00	39.11
ATOM	1311	CG	LYS	472	25.050	17.050	5.138	1.00	41.47
ATOM	1312	CD	LYS	472	26.080	17.957	5.794	1.00	46.97
ATOM	1313	CE	LYS	472	27.445	17.286	5.862	1.00	48.40
ATOM	1314	NZ	LYS	472	27.850	16.702	4.547	1.00	51.55
ATOM	1315	C	LYS	472	21.237	17.523	5.582	1.00	34.78
ATOM	1316	O	LYS	472	20.795	17.607	6.724	1.00	33.95
ATOM	1317	N	ASP	473	20.643	18.097	4.545	1.00	33.47
ATOM	1318	CA	ASP	473	19.420	18.865	4.720	1.00	34.63
ATOM	1319	CB	ASP	473	18.923	19.404	3.380	1.00	37.21
ATOM	1320	CG	ASP	473	17.654	20.221	3.522	1.00	43.24
ATOM	1321	OD1	ASP	473	16.559	19.687	3.230	1.00	45.20
ATOM	1322	OD2	ASP	473	17.750	21.396	3.932	1.00	45.59
ATOM	1323	C	ASP	473	18.339	17.998	5.338	1.00	32.93
ATOM	1324	O	ASP	473	17.642	18.416	6.264	1.00	32.87
ATOM	1325	N	HIS	474	18.199	16.784	4.827	1.00	32.74
ATOM	1326	CA	HIS	474	17.185	15.882	5.343	1.00	32.21
ATOM	1327	CB	HIS	474	17.185	14.575	4.568	1.00	32.79
ATOM	1328	CG	HIS	474	16.047	13.675	4.924	1.00	36.22
ATOM	1329	CD2	HIS	474	14.711	13.813	4.750	1.00	38.33
ATOM	1330	ND1	HIS	474	16.227	12.456	5.542	1.00	38.97
ATOM	1331	CE1	HIS	474	15.053	11.883	5.732	1.00	37.99

ATOM	1332	NE2	HIS	474	14.116	12.686	5.261	1.00	37.43
ATOM	1333	C	HIS	474	17.403	15.573	6.815	1.00	29.74
ATOM	1334	O	HIS	474	16.460	15.543	7.596	1.00	29.90
ATOM	1335	N	ILE	475	18.653	15.326	7.185	1.00	27.80
ATOM	1336	CA	ILE	475	18.971	15.014	8.571	1.00	25.61
ATOM	1337	CB	ILE	475	20.478	14.708	8.720	1.00	25.59
ATOM	1338	CG2	ILE	475	20.877	14.713	10.193	1.00	27.17
ATOM	1339	CG1	ILE	475	20.787	13.341	8.092	1.00	26.17
ATOM	1340	CD1	ILE	475	22.258	13.071	7.849	1.00	27.07
ATOM	1341	C	ILE	475	18.576	16.201	9.460	1.00	27.91
ATOM	1342	O	ILE	475	17.928	16.038	10.485	1.00	29.16
ATOM	1343	N	HIS	476	18.956	17.404	9.054	1.00	29.41
ATOM	1344	CA	HIS	476	18.621	18.575	9.846	1.00	29.73
ATOM	1345	CB	HIS	476	19.342	19.796	9.281	1.00	32.27
ATOM	1346	CG	HIS	476	20.777	19.867	9.699	1.00	39.44
ATOM	1347	CD2	HIS	476	21.355	19.707	10.915	1.00	39.81
ATOM	1348	ND1	HIS	476	21.809	20.067	8.808	1.00	39.79
ATOM	1349	CE1	HIS	476	22.959	20.027	9.456	1.00	39.98
ATOM	1350	NE2	HIS	476	22.712	19.809	10.735	1.00	40.26
ATOM	1351	C	HIS	476	17.120	18.810	9.948	1.00	31.40
ATOM	1352	O	HIS	476	16.636	19.336	10.951	1.00	29.79
ATOM	1353	N	ARG	477	16.374	18.396	8.929	1.00	31.82
ATOM	1354	CA	ARG	477	14.929	18.570	8.956	1.00	31.53
ATOM	1355	CB	ARG	477	14.343	18.376	7.557	1.00	34.95
ATOM	1356	CG	ARG	477	14.425	19.627	6.700	1.00	40.46
ATOM	1357	CD	ARG	477	13.698	19.445	5.370	1.00	45.22
ATOM	1358	NE	ARG	477	14.107	20.456	4.399	1.00	53.05
ATOM	1359	CZ	ARG	477	13.647	21.705	4.376	1.00	55.89
ATOM	1360	NH1	ARG	477	12.756	22.106	5.274	1.00	56.17
ATOM	1361	NH2	ARG	477	14.084	22.558	3.457	1.00	59.49
ATOM	1362	C	ARG	477	14.310	17.582	9.931	1.00	30.70
ATOM	1363	O	ARG	477	13.360	17.903	10.649	1.00	30.24
ATOM	1364	N	VAL	478	14.863	16.375	9.972	1.00	29.67
ATOM	1365	CA	VAL	478	14.351	15.369	10.887	1.00	29.68
ATOM	1366	CB	VAL	478	14.937	13.975	10.575	1.00	32.01
ATOM	1367	CG1	VAL	478	14.461	12.973	11.609	1.00	32.93
ATOM	1368	CG2	VAL	478	14.506	13.528	9.169	1.00	31.00
ATOM	1369	C	VAL	478	14.696	15.774	12.316	1.00	29.81
ATOM	1370	O	VAL	478	13.860	15.677	13.220	1.00	30.25
ATOM	1371	N	LEU	479	15.929	16.232	12.516	1.00	28.81
ATOM	1372	CA	LEU	479	16.360	16.674	13.836	1.00	28.74
ATOM	1373	CB	LEU	479	17.799	17.210	13.779	1.00	26.65
ATOM	1374	CG	LEU	479	18.910	16.152	13.853	1.00	26.05
ATOM	1375	CD1	LEU	479	20.231	16.772	13.395	1.00	25.81
ATOM	1376	CD2	LEU	479	19.028	15.603	15.277	1.00	25.34
ATOM	1377	C	LEU	479	15.411	17.777	14.313	1.00	29.54
ATOM	1378	O	LEU	479	14.997	17.786	15.472	1.00	29.00
ATOM	1379	N	ASP	480	15.076	18.703	13.415	1.00	31.52

ATOM	1380	CA	ASP	480	14.162	19.800	13.741	1.00	33.84
ATOM	1381	CB	ASP	480	13.943	20.712	12.528	1.00	34.37
ATOM	1382	CG	ASP	480	15.055	21.743	12.345	1.00	36.26
ATOM	1383	OD1	ASP	480	15.119	22.354	11.257	1.00	36.56
ATOM	1384	OD2	ASP	480	15.860	21.951	13.274	1.00	34.19
ATOM	1385	C	ASP	480	12.818	19.222	14.174	1.00	33.48
ATOM	1386	O	ASP	480	12.186	19.724	15.105	1.00	33.89
ATOM	1387	N	LYS	481	12.379	18.161	13.498	1.00	33.90
ATOM	1388	CA	LYS	481	11.106	17.536	13.839	1.00	32.97
ATOM	1389	CB	LYS	481	10.719	16.489	12.784	1.00	34.66
ATOM	1390	C	LYS	481	11.164	16.895	15.225	1.00	33.57
ATOM	1391	O	LYS	481	10.167	16.869	15.943	1.00	35.37
ATOM	1392	N	ILE	482	12.328	16.377	15.607	1.00	32.71
ATOM	1393	CA	ILE	482	12.457	15.764	16.922	1.00	31.60
ATOM	1394	CB	ILE	482	13.743	14.913	17.028	1.00	32.65
ATOM	1395	CG2	ILE	482	13.877	14.338	18.430	1.00	32.50
ATOM	1396	CG1	ILE	482	13.697	13.785	15.995	1.00	32.72
ATOM	1397	CD1	ILE	482	14.978	12.969	15.908	1.00	33.37
ATOM	1398	C	ILE	482	12.456	16.853	17.994	1.00	31.69
ATOM	1399	O	ILE	482	11.946	16.649	19.097	1.00	29.98
ATOM	1400	N	THR	483	13.027	18.012	17.679	1.00	31.33
ATOM	1401	CA	THR	483	13.022	19.109	18.644	1.00	31.71
ATOM	1402	CB	THR	483	13.756	20.351	18.109	1.00	32.92
ATOM	1403	OG1	THR	483	15.111	20.012	17.788	1.00	29.99
ATOM	1404	CG2	THR	483	13.756	21.452	19.160	1.00	30.47
ATOM	1405	C	THR	483	11.559	19.483	18.920	1.00	32.85
ATOM	1406	O	THR	483	11.146	19.598	20.070	1.00	31.83
ATOM	1407	N	ASP	484	10.785	19.656	17.851	1.00	31.91
ATOM	1408	CA	ASP	484	9.369	20.003	17.965	1.00	34.15
ATOM	1409	CB	ASP	484	8.708	20.013	16.591	1.00	37.41
ATOM	1410	CG	ASP	484	9.270	21.080	15.680	1.00	42.02
ATOM	1411	OD1	ASP	484	9.871	22.045	16.198	1.00	43.26
ATOM	1412	OD2	ASP	484	9.106	20.952	14.445	1.00	42.49
ATOM	1413	C	ASP	484	8.657	18.985	18.840	1.00	33.16
ATOM	1414	O	ASP	484	7.830	19.339	19.676	1.00	34.86
ATOM	1415	N	THR	485	8.996	17.715	18.646	1.00	33.91
ATOM	1416	CA	THR	485	8.396	16.635	19.414	1.00	34.41
ATOM	1417	CB	THR	485	8.875	15.268	18.885	1.00	33.58
ATOM	1418	OG1	THR	485	8.400	15.094	17.542	1.00	37.04
ATOM	1419	CG2	THR	485	8.347	14.138	19.751	1.00	30.89
ATOM	1420	C	THR	485	8.708	16.757	20.903	1.00	35.15
ATOM	1421	O	THR	485	7.818	16.600	21.744	1.00	31.99
ATOM	1422	N	LEU	486	9.966	17.046	21.229	1.00	33.77
ATOM	1423	CA	LEU	486	10.368	17.192	22.621	1.00	34.31
ATOM	1424	CB	LEU	486	11.879	17.448	22.721	1.00	32.00
ATOM	1425	CG	LEU	486	12.776	16.201	22.754	1.00	34.99
ATOM	1426	CD1	LEU	486	14.233	16.613	22.521	1.00	32.65
ATOM	1427	CD2	LEU	486	12.635	15.481	24.105	1.00	29.90

	ATOM	1428	C	LEU	486	9.597	18.348	23.256	1.00	34.87
	ATOM	1429	O	LEU	486	9.078	18.225	24.362	1.00	35.85
	ATOM	1430	N	ILE	487	9.513	19.469	22.548	1.00	35.59
	ATOM	1431	CA	ILE	487	8.787	20.625	23.064	1.00	36.79
	ATOM	1432	CB	ILE	487	8.890	21.826	22.095	1.00	37.32
	ATOM	1433	CG2	ILE	487	7.833	22.884	22.443	1.00	40.19
	ATOM	1434	CG1	ILE	487	10.292	22.443	22.181	1.00	36.00
	ATOM	1435	CD1	ILE	487	10.635	23.041	23.544	1.00	33.58
	ATOM	1436	C	ILE	487	7.315	20.257	23.276	1.00	38.56
	ATOM	1437	O	ILE	487	6.708	20.628	24.282	1.00	38.52
	ATOM	1438	N	HIS	488	6.749	19.521	22.326	1.00	40.33
	ATOM	1439	CA	HIS	488	5.357	19.096	22.427	1.00	42.29
	ATOM	1440	CB	HIS	488	4.962	18.282	21.197	1.00	44.26
	ATOM	1441	CG	HIS	488	3.612	17.647	21.305	1.00	47.75
	ATOM	1442	CD2	HIS	488	2.369	18.175	21.214	1.00	47.46
	ATOM	1443	ND1	HIS	488	3.440	16.298	21.534	1.00	51.09
	ATOM	1444	CE1	HIS	488	2.148	16.023	21.577	1.00	51.15
	ATOM	1445	NE2	HIS	488	1.477	17.144	21.385	1.00	50.22
	ATOM	1446	C	HIS	488	5.154	18.254	23.685	1.00	42.55
	ATOM	1447	O	HIS	488	4.233	18.498	24.467	1.00	43.02
	ATOM	1448	N	LEU	489	6.022	17.266	23.879	1.00	39.91
	ATOM	1449	CA	LEU	489	5.936	16.399	25.048	1.00	39.93
	ATOM	1450	CB	LEU	489	7.087	15.396	25.048	1.00	38.83
	ATOM	1451	CG	LEU	489	6.961	14.242	24.056	1.00	39.31
	ATOM	1452	CD1	LEU	489	8.259	13.456	24.027	1.00	39.01
	ATOM	1453	CD2	LEU	489	5.799	13.345	24.459	1.00	41.98
	ATOM	1454	C	LEU	489	5.973	17.203	26.339	1.00	40.24
	ATOM	1455	O	LEU	489	5.267	16.888	27.298	1.00	38.72
	ATOM	1456	N	MET	490	6.798	18.246	26.353	1.00	39.94
	ATOM	1457	CA	MET	490	6.939	19.102	27.522	1.00	41.50
	ATOM	1458	CB	MET	490	8.208	19.953	27.394	1.00	39.15
	ATOM	1459	CG	MET	490	9.495	19.169	27.608	1.00	41.69
	ATOM	1460	SD	MET	490	10.978	20.106	27.161	1.00	35.76
	ATOM	1461	CE	MET	490	12.178	18.775	27.056	1.00	39.22
	ATOM	1462	C	MET	490	5.718	20.004	27.717	1.00	42.33
	ATOM	1463	O	MET	490	5.296	20.258	28.848	1.00	41.09
	ATOM	1464	N	ALA	491	5.162	20.498	26.616	1.00	43.15
	ATOM	1465	CA	ALA	491	3.983	21.351	26.693	1.00	43.79
	ATOM	1466	CB	ALA	491	3.622	21.879	25.311	1.00	43.93
	ATOM	1467	C	ALA	491	2.841	20.510	27.251	1.00	46.16
	ATOM	1468	O	ALA	491	2.073	20.967	28.095	1.00	44.69
	ATOM	1469	N	LYS	492	2.752	19.268	26.783	1.00	46.29
	ATOM	1470	CA	LYS	492	1.711	18.351	27.222	1.00	49.90
	ATOM	1471	CB	LYS	492	1.772	17.053	26.411	1.00	50.03
	ATOM	1472	CG	LYS	492	1.087	17.135	25.062	1.00	53.81
	ATOM	1473	CD	LYS	492	-0.002	16.084	24.930	1.00	59.00
	ATOM	1474	CE	LYS	492	-0.988	16.453	23.827	1.00	61.85
	ATOM	1475	NZ	LYS	492	-1.351	15.281	22.976	1.00	62.89

ATOM	1476	C	LYS	492	1.841	18.025	28.701	1.00	51.15
ATOM	1477	O	LYS	492	0.845	17.784	29.379	1.00	53.37
ATOM	1478	N	ALA	493	3.072	18.012	29.199	1.00	50.15
ATOM	1479	CA	ALA	493	3.321	17.706	30.600	1.00	49.17
ATOM	1480	CB	ALA	493	4.777	17.314	30.794	1.00	50.39
ATOM	1481	C	ALA	493	2.971	18.885	31.501	1.00	49.36
ATOM	1482	O	ALA	493	3.089	18.799	32.723	1.00	51.57
ATOM	1483	N	GLY	494	2.554	19.989	30.893	1.00	48.61
ATOM	1484	CA	GLY	494	2.185	21.159	31.671	1.00	46.92
ATOM	1485	C	GLY	494	3.322	22.107	32.006	1.00	45.46
ATOM	1486	O	GLY	494	3.206	22.921	32.919	1.00	43.58
ATOM	1487	N	LEU	495	4.431	22.009	31.284	1.00	44.81
ATOM	1488	CA	LEU	495	5.555	22.899	31.540	1.00	42.34
ATOM	1489	CB	LEU	495	6.847	22.293	30.988	1.00	43.79
ATOM	1490	CG	LEU	495	7.712	21.459	31.936	1.00	40.99
ATOM	1491	CD1	LEU	495	7.022	20.156	32.260	1.00	44.70
ATOM	1492	CD2	LEU	495	9.072	21.189	31.270	1.00	42.12
ATOM	1493	C	LEU	495	5.278	24.227	30.847	1.00	42.13
ATOM	1494	O	LEU	495	4.664	24.258	29.778	1.00	42.49
ATOM	1495	N	THR	496	5.718	25.324	31.452	1.00	42.73
ATOM	1496	CA	THR	496	5.521	26.636	30.845	1.00	43.56
ATOM	1497	CB	THR	496	5.841	27.767	31.829	1.00	46.09
ATOM	1498	OG1	THR	496	7.222	27.688	32.208	1.00	43.92
ATOM	1499	CG2	THR	496	4.965	27.662	33.064	1.00	45.63
ATOM	1500	C	THR	496	6.471	26.764	29.660	1.00	45.54
ATOM	1501	O	THR	496	7.370	25.939	29.488	1.00	43.39
ATOM	1502	N	LEU	497	6.280	27.800	28.849	1.00	45.02
ATOM	1503	CA	LEU	497	7.135	28.020	27.688	1.00	45.12
ATOM	1504	CB	LEU	497	6.710	29.286	26.944	1.00	46.62
ATOM	1505	CG	LEU	497	5.933	29.080	25.640	1.00	50.20
ATOM	1506	CD1	LEU	497	5.886	30.397	24.875	1.00	50.95
ATOM	1507	CD2	LEU	497	6.589	27.990	24.798	1.00	50.91
ATOM	1508	C	LEU	497	8.599	28.135	28.101	1.00	44.94
ATOM	1509	O	LEU	497	9.474	27.516	27.493	1.00	45.03
ATOM	1510	N	GLN	498	8.862	28.927	29.137	1.00	41.14
ATOM	1511	CA	GLN	498	10.221	29.101	29.627	1.00	40.54
ATOM	1512	CB	GLN	498	10.246	30.140	30.743	1.00	43.82
ATOM	1513	CG	GLN	498	11.585	30.270	31.437	1.00	43.37
ATOM	1514	CD	GLN	498	11.539	31.260	32.584	1.00	47.03
ATOM	1515	OE1	GLN	498	10.565	31.308	33.332	1.00	49.18
ATOM	1516	NE2	GLN	498	12.591	32.054	32.727	1.00	45.30
ATOM	1517	C	GLN	498	10.777	27.773	30.145	1.00	39.39
ATOM	1518	O	GLN	498	11.923	27.422	29.866	1.00	35.05
ATOM	1519	N	GLN	499	9.965	27.040	30.902	1.00	36.49
ATOM	1520	CA	GLN	499	10.391	25.748	31.434	1.00	36.91
ATOM	1521	CB	GLN	499	9.314	25.155	32.344	1.00	38.84
ATOM	1522	CG	GLN	499	9.155	25.825	33.703	1.00	41.33
ATOM	1523	CD	GLN	499	8.039	25.187	34.512	1.00	42.74

	ATOM	1524	OE1	GLN	499	7.027	24.760	33.955	1.00	45.44
	ATOM	1525	NE2	GLN	499	8.222	25.107	35.829	1.00	43.48
	ATOM	1526	C	GLN	499	10.655	24.773	30.285	1.00	35.03
	ATOM	1527	O	GLN	499	11.446	23.832	30.422	1.00	36.59
	ATOM	1528	N	GLN	500	9.980	24.994	29.162	1.00	34.14
	ATOM	1529	CA	GLN	500	10.136	24.138	27.990	1.00	34.65
	ATOM	1530	CB	GLN	500	9.042	24.436	26.958	1.00	33.90
	ATOM	1531	CG	GLN	500	7.672	23.872	27.315	1.00	36.62
	ATOM	1532	CD	GLN	500	6.558	24.419	26.435	1.00	40.17
	ATOM	1533	OE1	GLN	500	6.660	24.417	25.207	1.00	40.22
	ATOM	1534	NE2	GLN	500	5.482	24.886	27.064	1.00	41.82
	ATOM	1535	C	GLN	500	11.511	24.350	27.358	1.00	34.96
	ATOM	1536	O	GLN	500	12.256	23.387	27.124	1.00	30.79
	ATOM	1537	N	HIS	501	11.835	25.612	27.078	1.00	34.21
	ATOM	1538	CA	HIS	501	13.117	25.966	26.480	1.00	37.42
	ATOM	1539	CB	HIS	501	13.195	27.476	26.246	1.00	43.08
	ATOM	1540	CG	HIS	501	12.043	28.027	25.468	1.00	51.13
	ATOM	1541	CD2	HIS	501	11.534	27.678	24.263	1.00	53.05
	ATOM	1542	ND1	HIS	501	11.264	29.068	25.926	1.00	54.54
	ATOM	1543	CE1	HIS	501	10.325	29.337	25.037	1.00	54.36
	ATOM	1544	NE2	HIS	501	10.466	28.508	24.018	1.00	55.19
	ATOM	1545	C	HIS	501	14.255	25.543	27.395	1.00	35.79
	ATOM	1546	O	HIS	501	15.271	24.996	26.945	1.00	36.20
	ATOM	1547	N	GLN	502	14.086	25.799	28.685	1.00	33.90
	ATOM	1548	CA	GLN	502	15.110	25.438	29.650	1.00	32.18
	ATOM	1549	CB	GLN	502	14.740	25.977	31.033	1.00	35.84
	ATOM	1550	CG	GLN	502	14.787	27.498	31.113	1.00	32.66
	ATOM	1551	CD	GLN	502	14.420	28.028	32.486	1.00	36.62
	ATOM	1552	OE1	GLN	502	14.102	27.262	33.397	1.00	33.99
	ATOM	1553	NE2	GLN	502	14.462	29.348	32.640	1.00	36.22
	ATOM	1554	C	GLN	502	15.340	23.932	29.716	1.00	31.79
	ATOM	1555	O	GLN	502	16.483	23.479	29.769	1.00	28.00
	ATOM	1556	N	ARG	503	14.266	23.146	29.705	1.00	30.99
	ATOM	1557	CA	ARG	503	14.436	21.704	29.779	1.00	29.91
	ATOM	1558	CB	ARG	503	13.107	21.011	30.052	1.00	32.79
	ATOM	1559	CG	ARG	503	13.258	19.541	30.400	1.00	30.84
	ATOM	1560	CD	ARG	503	11.930	18.935	30.798	1.00	30.61
	ATOM	1561	NE	ARG	503	12.021	17.490	30.992	1.00	28.50
	ATOM	1562	CZ	ARG	503	12.489	16.908	32.093	1.00	29.00
	ATOM	1563	NH1	ARG	503	12.917	17.640	33.114	1.00	29.85
	ATOM	1564	NH2	ARG	503	12.512	15.583	32.180	1.00	33.73
	ATOM	1565	C	ARG	503	15.051	21.152	28.496	1.00	29.89
	ATOM	1566	O	ARG	503	15.895	20.259	28.548	1.00	29.69
	ATOM	1567	N	LEU	504	14.624	21.675	27.351	1.00	28.99
	ATOM	1568	CA	LEU	504	15.164	21.223	26.075	1.00	28.90
	ATOM	1569	CB	LEU	504	14.566	22.023	24.916	1.00	27.72
	ATOM	1570	CG	LEU	504	15.327	21.901	23.593	1.00	30.47
	ATOM	1571	CD1	LEU	504	15.252	20.453	23.117	1.00	31.74

ATOM	1572	CD2	LEU	504	14.742	22.843	22.542	1.00	29.85
ATOM	1573	C	LEU	504	16.681	21.419	26.089	1.00	29.69
ATOM	1574	O	LEU	504	17.439	20.536	25.672	1.00	26.38
ATOM	1575	N	ALA	505	17.114	22.585	26.564	1.00	28.51
ATOM	1576	CA	ALA	505	18.535	22.899	26.632	1.00	25.98
ATOM	1577	CB	ALA	505	18.735	24.361	27.039	1.00	29.86
ATOM	1578	C	ALA	505	19.261	21.977	27.604	1.00	26.67
ATOM	1579	O	ALA	505	20.340	21.462	27.290	1.00	25.54
ATOM	1580	N	GLN	506	18.677	21.771	28.784	1.00	23.59
ATOM	1581	CA	GLN	506	19.299	20.907	29.785	1.00	27.67
ATOM	1582	CB	GLN	506	18.434	20.796	31.043	1.00	27.75
ATOM	1583	CG	GLN	506	18.414	22.027	31.945	1.00	32.48
ATOM	1584	CD	GLN	506	17.111	22.116	32.736	1.00	38.40
ATOM	1585	OE1	GLN	506	16.319	21.167	32.754	1.00	35.97
ATOM	1586	NE2	GLN	506	16.879	23.257	33.386	1.00	38.07
ATOM	1587	C	GLN	506	19.500	19.509	29.217	1.00	24.53
ATOM	1588	O	GLN	506	20.536	18.889	29.441	1.00	26.42
ATOM	1589	N	LEU	507	18.505	19.017	28.484	1.00	26.78
ATOM	1590	CA	LEU	507	18.578	17.678	27.902	1.00	26.18
ATOM	1591	CB	LEU	507	17.225	17.286	27.295	1.00	31.48
ATOM	1592	CG	LEU	507	16.052	16.961	28.231	1.00	32.59
ATOM	1593	CD1	LEU	507	14.836	16.561	27.389	1.00	33.78
ATOM	1594	CD2	LEU	507	16.431	15.838	29.174	1.00	30.18
ATOM	1595	C	LEU	507	19.652	17.583	26.819	1.00	26.03
ATOM	1596	O	LEU	507	20.421	16.621	26.771	1.00	27.28
ATOM	1597	N	LEU	508	19.713	18.583	25.950	1.00	24.31
ATOM	1598	CA	LEU	508	20.690	18.557	24.863	1.00	23.68
ATOM	1599	CB	LEU	508	20.339	19.629	23.828	1.00	23.91
ATOM	1600	CG	LEU	508	19.004	19.436	23.102	1.00	24.68
ATOM	1601	CD1	LEU	508	18.905	20.416	21.945	1.00	25.11
ATOM	1602	CD2	LEU	508	18.903	17.994	22.580	1.00	27.53
ATOM	1603	C	LEU	508	22.127	18.727	25.341	1.00	22.93
ATOM	1604	O	LEU	508	23.062	18.200	24.736	1.00	21.36
ATOM	1605	N	LEU	509	22.302	19.451	26.441	1.00	23.86
ATOM	1606	CA	LEU	509	23.637	19.661	26.991	1.00	26.28
ATOM	1607	CB	LEU	509	23.598	20.735	28.095	1.00	28.08
ATOM	1608	CG	LEU	509	23.578	22.214	27.672	1.00	33.98
ATOM	1609	CD1	LEU	509	23.529	23.114	28.921	1.00	35.23
ATOM	1610	CD2	LEU	509	24.818	22.525	26.856	1.00	30.48
ATOM	1611	C	LEU	509	24.154	18.327	27.540	1.00	26.08
ATOM	1612	O	LEU	509	25.354	18.068	27.547	1.00	23.92
ATOM	1613	N	ILE	510	23.254	17.462	27.993	1.00	24.60
ATOM	1614	CA	ILE	510	23.712	16.172	28.496	1.00	25.12
ATOM	1615	CB	ILE	510	22.568	15.368	29.161	1.00	28.51
ATOM	1616	CG2	ILE	510	23.051	13.965	29.506	1.00	31.67
ATOM	1617	CG1	ILE	510	22.141	16.060	30.459	1.00	31.18
ATOM	1618	CD1	ILE	510	20.712	15.749	30.882	1.00	37.16
ATOM	1619	C	ILE	510	24.337	15.351	27.364	1.00	23.86

	ATOM	1620	O	ILE	510	25.225	14.534	27.600	1.00	24.14
	ATOM	1621	N	LEU	511	23.889	15.586	26.133	1.00	25.10
	ATOM	1622	CA	LEU	511	24.420	14.862	24.977	1.00	25.63
	ATOM	1623	CB	LEU	511	23.628	15.225	23.714	1.00	23.89
5	ATOM	1624	CG	LEU	511	22.152	14.801	23.659	1.00	25.78
	ATOM	1625	CD1	LEU	511	21.648	14.920	22.224	1.00	26.55
	ATOM	1626	CD2	LEU	511	21.990	13.363	24.146	1.00	26.29
	ATOM	1627	C	LEU	511	25.912	15.152	24.771	1.00	27.10
	ATOM	1628	O	LEU	511	26.641	14.332	24.214	1.00	24.98
10	ATOM	1629	N	SER	512	26.372	16.319	25.213	1.00	24.75
	ATOM	1630	CA	SER	512	27.787	16.637	25.076	1.00	23.68
	ATOM	1631	CB	SER	512	28.023	18.129	25.358	1.00	26.12
	ATOM	1632	OG	SER	512	29.271	18.327	25.986	1.00	37.17
	ATOM	1633	C	SER	512	28.594	15.765	26.050	1.00	23.15
15	ATOM	1634	O	SER	512	29.742	15.383	25.769	1.00	22.15
	ATOM	1635	N	AHIS	513	27.993	15.456	27.192	0.50	21.53
	ATOM	1636	N	BHIS	513	28.008	15.453	27.202	0.50	20.99
	ATOM	1637	CA	AHIS	513	28.645	14.624	28.196	0.50	21.79
	ATOM	1638	CA	BHIS	513	28.696	14.607	28.174	0.50	20.94
20	ATOM	1639	CB	AHIS	513	27.920	14.776	29.536	0.50	23.59
	ATOM	1640	CB	BHIS	513	27.991	14.636	29.536	0.50	21.59
	ATOM	1641	CG	AHIS	513	28.145	16.109	30.179	0.50	27.34
	ATOM	1642	CG	BHIS	513	28.800	14.032	30.642	0.50	23.94
	ATOM	1643	CD2A	HIS	513	29.223	16.616	30.824	0.50	27.56
25	ATOM	1644	CD2B	HIS	513	30.095	14.211	31.001	0.50	24.22
	ATOM	1645	ND1A	HIS	513	27.204	17.117	30.160	0.50	30.62
	ATOM	1646	ND1B	HIS	513	28.285	13.105	31.523	0.50	27.00
	ATOM	1647	CE1A	HIS	513	27.693	18.185	30.763	0.50	26.32
	ATOM	1648	CE1B	HIS	513	29.225	12.740	32.376	0.50	24.40
30	ATOM	1649	NE2A	HIS	513	28.916	17.908	31.176	0.50	28.30
	ATOM	1650	NE2B	HIS	513	30.334	13.396	32.081	0.50	25.54
	ATOM	1651	C	AHIS	513	28.666	13.164	27.738	0.50	19.81
	ATOM	1652	C	BHIS	513	28.720	13.171	27.652	0.50	19.42
	ATOM	1653	O	AHIS	513	29.601	12.426	28.026	0.50	22.45
35	ATOM	1654	O	BHIS	513	29.707	12.457	27.809	0.50	22.62
	ATOM	1655	N	ILE	514	27.633	12.753	27.015	1.00	20.76
	ATOM	1656	CA	ILE	514	27.572	11.396	26.492	1.00	20.94
	ATOM	1657	CB	ILE	514	26.154	11.086	25.953	1.00	27.76
	ATOM	1658	CG2	ILE	514	26.169	9.800	25.123	1.00	28.26
40	ATOM	1659	CG1	ILE	514	25.185	10.965	27.139	1.00	27.91
	ATOM	1660	CD1	ILE	514	23.752	10.649	26.753	1.00	34.31
	ATOM	1661	C	ILE	514	28.641	11.256	25.398	1.00	20.66
	ATOM	1662	O	ILE	514	29.298	10.226	25.285	1.00	22.21
	ATOM	1663	N	ARG	515	28.825	12.294	24.589	1.00	20.48
45	ATOM	1664	CA	ARG	515	29.861	12.243	23.554	1.00	21.98
	ATOM	1665	CB	ARG	515	29.861	13.535	22.726	1.00	23.11
	ATOM	1666	CG	ARG	515	31.003	13.611	21.737	1.00	25.76
	ATOM	1667	CD	ARG	515	30.664	12.818	20.491	1.00	28.55

ATOM	1668	NE	ARG	515	29.580	13.482	19.788	1.00	36.24
ATOM	1669	CZ	ARG	515	29.615	13.827	18.508	1.00	38.91
ATOM	1670	NH1	ARG	515	30.689	13.566	17.776	1.00	35.37
ATOM	1671	NH2	ARG	515	28.579	14.459	17.971	1.00	40.27
ATOM	1672	C	ARG	515	31.221	12.087	24.225	1.00	21.29
ATOM	1673	O	ARG	515	32.068	11.305	23.795	1.00	20.06
ATOM	1674	N	HIS	516	31.420	12.844	25.293	1.00	23.23
ATOM	1675	CA	HIS	516	32.675	12.812	26.034	1.00	24.75
ATOM	1676	CB	HIS	516	32.566	13.794	27.206	1.00	24.03
ATOM	1677	CG	HIS	516	33.826	13.948	27.990	1.00	31.42
ATOM	1678	CD2	HIS	516	34.138	13.587	29.257	1.00	35.87
ATOM	1679	ND1	HIS	516	34.938	14.586	27.489	1.00	33.59
ATOM	1680	CE1	HIS	516	35.882	14.613	28.411	1.00	35.70
ATOM	1681	NE2	HIS	516	35.422	14.013	29.495	1.00	33.35
ATOM	1682	C	HIS	516	32.965	11.390	26.537	1.00	24.02
ATOM	1683	O	HIS	516	34.059	10.852	26.362	1.00	23.66
ATOM	1684	N	MET	517	31.969	10.786	27.168	1.00	20.91
ATOM	1685	CA	MET	517	32.109	9.436	27.684	1.00	24.21
ATOM	1686	CB	MET	517	30.837	9.038	28.424	1.00	23.88
ATOM	1687	CG	MET	517	30.607	9.903	29.652	1.00	26.32
ATOM	1688	SD	MET	517	29.435	9.222	30.790	1.00	26.67
ATOM	1689	CE	MET	517	27.914	9.390	29.807	1.00	23.26
ATOM	1690	C	MET	517	32.399	8.448	26.564	1.00	23.26
ATOM	1691	O	MET	517	33.213	7.547	26.728	1.00	26.08
ATOM	1692	N	SER	518	31.736	8.612	25.423	1.00	21.93
ATOM	1693	CA	SER	518	31.977	7.717	24.301	1.00	23.08
ATOM	1694	CB	SER	518	30.976	8.027	23.173	1.00	22.02
ATOM	1695	OG	SER	518	31.283	7.336	21.978	1.00	24.01
ATOM	1696	C	SER	518	33.432	7.862	23.810	1.00	25.15
ATOM	1697	O	SER	518	34.111	6.866	23.532	1.00	22.94
ATOM	1698	N	ASN	519	33.923	9.097	23.713	1.00	22.42
ATOM	1699	CA	ASN	519	35.295	9.309	23.260	1.00	21.87
ATOM	1700	CB	ASN	519	35.605	10.807	23.157	1.00	24.46
ATOM	1701	CG	ASN	519	34.864	11.469	22.021	1.00	29.02
ATOM	1702	OD1	ASN	519	34.661	10.864	20.965	1.00	31.93
ATOM	1703	ND2	ASN	519	34.459	12.715	22.224	1.00	28.81
ATOM	1704	C	ASN	519	36.292	8.643	24.201	1.00	21.46
ATOM	1705	O	ASN	519	37.251	8.015	23.752	1.00	23.56
ATOM	1706	N	LYS	520	36.070	8.782	25.504	1.00	23.23
ATOM	1707	CA	LYS	520	36.964	8.171	26.488	1.00	26.35
ATOM	1708	CB	LYS	520	36.581	8.592	27.912	1.00	27.53
ATOM	1709	CG	LYS	520	36.618	10.101	28.174	1.00	33.74
ATOM	1710	CD	LYS	520	37.962	10.710	27.811	1.00	42.09
ATOM	1711	CE	LYS	520	39.047	10.307	28.802	1.00	43.97
ATOM	1712	NZ	LYS	520	39.858	11.480	29.254	1.00	48.07
ATOM	1713	C	LYS	520	36.899	6.644	26.376	1.00	27.71
ATOM	1714	O	LYS	520	37.913	5.957	26.501	1.00	27.15
ATOM	1715	N	GLY	521	35.704	6.117	26.141	1.00	25.02

ATOM	1716	CA	GLY	521	35.562	4.676	26.003	1.00	26.67
ATOM	1717	C	GLY	521	36.254	4.168	24.753	1.00	27.06
ATOM	1718	O	GLY	521	36.924	3.128	24.775	1.00	26.84
ATOM	1719	N	AMET	522	36.101	4.893	23.650	0.50	25.87
ATOM	1720	N	BMET	522	36.095	4.908	23.658	0.50	27.62
ATOM	1721	CA	AMET	522	36.727	4.491	22.401	0.50	27.27
ATOM	1722	CA	BMET	522	36.703	4.551	22.384	0.50	30.14
ATOM	1723	CB	AMET	522	36.267	5.396	21.260	0.50	26.50
ATOM	1724	CB	BMET	522	36.252	5.525	21.288	0.50	32.46
ATOM	1725	CG	AMET	522	34.827	5.162	20.866	0.50	25.05
ATOM	1726	CG	BMET	522	35.681	4.854	20.045	0.50	35.70
ATOM	1727	SD	AMET	522	34.585	3.587	20.020	0.50	27.07
ATOM	1728	SD	BMET	522	34.197	5.672	19.408	0.50	40.01
ATOM	1729	CE	AMET	522	33.142	4.017	19.031	0.50	31.29
ATOM	1730	CE	BMET	522	34.733	6.085	17.745	0.50	42.12
ATOM	1731	C	AMET	522	38.242	4.532	22.512	0.50	28.99
ATOM	1732	C	BMET	522	38.224	4.567	22.483	0.50	30.76
ATOM	1733	O	AMET	522	38.939	3.743	21.870	0.50	31.65
ATOM	1734	O	BMET	522	38.905	3.793	21.807	0.50	32.87
ATOM	1735	N	GLU	523	38.749	5.452	23.324	1.00	30.85
ATOM	1736	CA	GLU	523	40.190	5.576	23.513	1.00	34.09
ATOM	1737	CB	GLU	523	40.515	6.725	24.480	1.00	35.59
ATOM	1738	CG	GLU	523	40.658	8.079	23.784	1.00	43.35
ATOM	1739	CD	GLU	523	40.560	9.265	24.739	1.00	46.63
ATOM	1740	OE1	GLU	523	39.832	10.240	24.416	1.00	47.64
ATOM	1741	OE2	GLU	523	41.212	9.225	25.805	1.00	43.09
ATOM	1742	C	GLU	523	40.718	4.260	24.061	1.00	34.62
ATOM	1743	O	GLU	523	41.733	3.747	23.596	1.00	33.87
ATOM	1744	N	HIS	524	40.021	3.700	25.042	1.00	36.33
ATOM	1745	CA	HIS	524	40.455	2.427	25.607	1.00	39.20
ATOM	1746	CB	HIS	524	39.678	2.093	26.878	1.00	40.75
ATOM	1747	CG	HIS	524	40.061	0.774	27.473	1.00	48.10
ATOM	1748	CD2	HIS	524	41.192	0.376	28.104	1.00	48.56
ATOM	1749	ND1	HIS	524	39.247	-0.338	27.412	1.00	48.84
ATOM	1750	CE1	HIS	524	39.859	-1.362	27.978	1.00	50.19
ATOM	1751	NE2	HIS	524	41.041	-0.956	28.407	1.00	51.61
ATOM	1752	C	HIS	524	40.290	1.282	24.613	1.00	38.06
ATOM	1753	O	HIS	524	41.226	0.521	24.371	1.00	38.18
ATOM	1754	N	LEU	525	39.101	1.162	24.034	1.00	36.96
ATOM	1755	CA	LEU	525	38.831	0.093	23.084	1.00	37.40
ATOM	1756	CB	LEU	525	37.416	0.241	22.514	1.00	35.89
ATOM	1757	CG	LEU	525	36.268	0.107	23.527	1.00	33.17
ATOM	1758	CD1	LEU	525	34.936	0.246	22.811	1.00	31.77
ATOM	1759	CD2	LEU	525	36.343	-1.240	24.238	1.00	35.92
ATOM	1760	C	LEU	525	39.859	0.057	21.954	1.00	41.32
ATOM	1761	O	LEU	525	40.244	-1.015	21.487	1.00	40.76
ATOM	1762	N	TYR	526	40.314	1.227	21.522	1.00	43.68
ATOM	1763	CA	TYR	526	41.300	1.297	20.449	1.00	49.00

	ATOM	1764	CB	TYR	526	41.376	2.722	19.890	1.00	51.86
	ATOM	1765	CG	TYR	526	42.305	2.878	18.704	1.00	57.70
	ATOM	1766	CD1	TYR	526	41.835	2.718	17.400	1.00	58.93
	ATOM	1767	CE1	TYR	526	42.681	2.875	16.305	1.00	61.21
	ATOM	1768	CD2	TYR	526	43.653	3.200	18.883	1.00	58.58
	ATOM	1769	CE2	TYR	526	44.510	3.359	17.790	1.00	61.15
	ATOM	1770	CZ	TYR	526	44.016	3.194	16.505	1.00	61.09
	ATOM	1771	OH	TYR	526	44.851	3.343	15.417	1.00	63.79
	ATOM	1772	C	TYR	526	42.671	0.871	20.964	1.00	50.14
	ATOM	1773	O	TYR	526	43.471	0.303	20.223	1.00	50.73
	ATOM	1774	N	SER	527	42.930	1.139	22.240	1.00	52.72
	ATOM	1775	CA	SER	527	44.205	0.790	22.857	1.00	55.88
	ATOM	1776	CB	SER	527	44.351	1.516	24.199	1.00	55.00
	ATOM	1777	OG	SER	527	43.752	0.788	25.257	1.00	52.46
	ATOM	1778	C	SER	527	44.365	-0.718	23.054	1.00	60.39
	ATOM	1779	O	SER	527	45.398	-1.185	23.534	1.00	60.43
	ATOM	1780	N	MET	528	43.335	-1.472	22.678	1.00	63.86
	ATOM	1781	CA	MET	528	43.347	-2.929	22.788	1.00	67.95
	ATOM	1782	CB	MET	528	42.534	-3.381	24.008	1.00	67.85
	ATOM	1783	CG	MET	528	41.237	-2.606	24.222	1.00	70.10
	ATOM	1784	SD	MET	528	39.895	-3.569	24.983	1.00	71.70
	ATOM	1785	CE	MET	528	39.231	-4.412	23.554	1.00	72.57
	ATOM	1786	C	MET	528	42.726	-3.502	21.513	1.00	70.33
	ATOM	1787	O	MET	528	42.170	-4.602	21.513	1.00	72.43
	ATOM	1788	N	LYS	529	42.834	-2.739	20.428	1.00	71.53
	ATOM	1789	CA	LYS	529	42.274	-3.122	19.136	1.00	72.00
	ATOM	1790	CB	LYS	529	42.508	-2.004	18.119	1.00	71.30
	ATOM	1791	C	LYS	529	42.813	-4.439	18.587	1.00	72.47
	ATOM	1792	O	LYS	529	43.990	-4.762	18.751	1.00	70.37
	ATOM	1793	N	CYS	530	41.932	-5.191	17.930	1.00	74.48
	ATOM	1794	CA	CYS	530	42.279	-6.474	17.325	1.00	76.67
	ATOM	1795	CB	CYS	530	41.004	-7.245	16.952	1.00	77.23
	ATOM	1796	SG	CYS	530	40.447	-8.491	18.146	1.00	79.38
	ATOM	1797	C	CYS	530	43.098	-6.220	16.065	1.00	78.08
	ATOM	1798	O	CYS	530	43.241	-5.076	15.623	1.00	78.81
	ATOM	1799	N	LYS	531	43.637	-7.289	15.487	1.00	78.22
	ATOM	1800	CA	LYS	531	44.424	-7.187	14.267	1.00	78.15
	ATOM	1801	CB	LYS	531	45.600	-8.182	14.305	1.00	78.33
	ATOM	1802	C	LYS	531	43.508	-7.467	13.067	1.00	77.93
	ATOM	1803	O	LYS	531	42.549	-6.734	12.839	1.00	78.07
	ATOM	1804	N	ASN	532	43.784	-8.539	12.328	1.00	77.80
	ATOM	1805	CA	ASN	532	42.984	-8.902	11.152	1.00	77.30
	ATOM	1806	CB	ASN	532	43.550	-10.166	10.521	1.00	77.55
	ATOM	1807	C	ASN	532	41.485	-9.082	11.423	1.00	77.34
	ATOM	1808	O	ASN	532	40.904	-10.123	11.118	1.00	78.13
	ATOM	1809	N	VAL	533	40.859	-8.055	11.988	1.00	76.13
	ATOM	1810	CA	VAL	533	39.436	-8.098	12.280	1.00	73.77
	ATOM	1811	CB	VAL	533	39.155	-7.715	13.752	1.00	73.62

	ATOM	1812	CG1	VAL	533	39.690	-6.327	14.047	1.00	73.13
	ATOM	1813	CG2	VAL	533	37.662	-7.782	14.021	1.00	73.14
	ATOM	1814	C	VAL	533	38.685	-7.143	11.352	1.00	72.97
	ATOM	1815	O	VAL	533	39.024	-5.960	11.252	1.00	73.91
	ATOM	1816	N	VAL	534	37.671	-7.666	10.666	1.00	70.02
	ATOM	1817	CA	VAL	534	36.866	-6.867	9.747	1.00	66.70
	ATOM	1818	CB	VAL	534	35.619	-7.646	9.328	1.00	67.32
	ATOM	1819	C	VAL	534	36.463	-5.541	10.393	1.00	63.87
	ATOM	1820	O	VAL	534	35.895	-5.519	11.486	1.00	63.55
	ATOM	1821	N	PRO	535	36.756	-4.415	9.719	1.00	60.92
	ATOM	1822	CD	PRO	535	37.424	-4.354	8.408	1.00	61.01
	ATOM	1823	CA	PRO	535	36.424	-3.077	10.229	1.00	56.83
	ATOM	1824	CB	PRO	535	36.867	-2.135	9.107	1.00	58.70
	ATOM	1825	CG	PRO	535	37.023	-3.009	7.893	1.00	61.55
	ATOM	1826	C	PRO	535	34.944	-2.902	10.571	1.00	52.90
	ATOM	1827	O	PRO	535	34.067	-3.461	9.908	1.00	52.01
	ATOM	1828	N	LEU	536	34.672	-2.120	11.610	1.00	48.60
	ATOM	1829	CA	LEU	536	33.301	-1.874	12.042	1.00	45.08
	ATOM	1830	CB	LEU	536	33.280	-0.796	13.128	1.00	44.35
	ATOM	1831	CG	LEU	536	32.267	-0.911	14.273	1.00	43.48
	ATOM	1832	CD1	LEU	536	31.919	0.490	14.745	1.00	43.41
	ATOM	1833	CD2	LEU	536	31.022	-1.654	13.835	1.00	39.55
	ATOM	1834	C	LEU	536	32.434	-1.433	10.871	1.00	43.58
	ATOM	1835	O	LEU	536	31.287	-1.862	10.734	1.00	42.14
	ATOM	1836	N	TYR	537	32.992	-0.575	10.024	1.00	43.02
	ATOM	1837	CA	TYR	537	32.269	-0.066	8.866	1.00	43.34
	ATOM	1838	CB	TYR	537	33.200	0.786	7.997	1.00	44.76
	ATOM	1839	CG	TYR	537	32.483	1.558	6.913	1.00	48.28
	ATOM	1840	CD1	TYR	537	32.190	0.964	5.687	1.00	48.46
	ATOM	1841	CE1	TYR	537	31.504	1.660	4.693	1.00	52.48
	ATOM	1842	CD2	TYR	537	32.073	2.875	7.123	1.00	49.99
	ATOM	1843	CE2	TYR	537	31.383	3.584	6.135	1.00	53.73
	ATOM	1844	CZ	TYR	537	31.100	2.967	4.924	1.00	54.01
	ATOM	1845	OH	TYR	537	30.401	3.648	3.952	1.00	55.90
	ATOM	1846	C	TYR	537	31.683	-1.199	8.032	1.00	43.15
	ATOM	1847	O	TYR	537	30.500	-1.191	7.696	1.00	41.54
	ATOM	1848	N	ASP	538	32.521	-2.175	7.702	1.00	44.67
	ATOM	1849	CA	ASP	538	32.097	-3.309	6.893	1.00	45.49
	ATOM	1850	CB	ASP	538	33.322	-4.126	6.479	1.00	51.32
	ATOM	1851	CG	ASP	538	34.361	-3.284	5.748	1.00	56.17
	ATOM	1852	OD1	ASP	538	35.436	-3.820	5.396	1.00	57.29
	ATOM	1853	OD2	ASP	538	34.097	-2.079	5.526	1.00	59.24
	ATOM	1854	C	ASP	538	31.071	-4.195	7.587	1.00	43.48
	ATOM	1855	O	ASP	538	30.177	-4.738	6.940	1.00	43.95
	ATOM	1856	N	LEU	539	31.193	-4.345	8.901	1.00	41.57
	ATOM	1857	CA	LEU	539	30.244	-5.157	9.654	1.00	39.11
	ATOM	1858	CB	LEU	539	30.734	-5.351	11.092	1.00	41.88
	ATOM	1859	CG	LEU	539	29.770	-6.065	12.044	1.00	46.11

	ATOM	1860	CD1	LEU	539	29.298	-7.379	11.423	1.00	46.99
	ATOM	1861	CD2	LEU	539	30.474	-6.319	13.377	1.00	45.76
	ATOM	1862	C	LEU	539	28.891	-4.451	9.651	1.00	36.38
	ATOM	1863	O	LEU	539	27.849	-5.070	9.436	1.00	35.74
5	ATOM	1864	N	LEU	540	28.919	-3.146	9.894	1.00	35.50
	ATOM	1865	CA	LEU	540	27.703	-2.336	9.903	1.00	35.59
	ATOM	1866	CB	LEU	540	28.061	-0.877	10.219	1.00	37.63
	ATOM	1867	CG	LEU	540	27.856	-0.252	11.605	1.00	40.28
	ATOM	1868	CD1	LEU	540	27.526	-1.299	12.645	1.00	38.55
10	ATOM	1869	CD2	LEU	540	29.114	0.506	11.985	1.00	41.04
	ATOM	1870	C	LEU	540	27.060	-2.415	8.510	1.00	35.50
	ATOM	1871	O	LEU	540	25.846	-2.585	8.371	1.00	33.21
	ATOM	1872	N	LEU	541	27.892	-2.289	7.483	1.00	37.01
	ATOM	1873	CA	LEU	541	27.418	-2.340	6.101	1.00	38.51
15	ATOM	1874	CB	LEU	541	28.591	-2.152	5.145	1.00	39.67
	ATOM	1875	CG	LEU	541	28.301	-2.112	3.643	1.00	40.92
	ATOM	1876	CD1	LEU	541	27.184	-1.130	3.348	1.00	42.44
	ATOM	1877	CD2	LEU	541	29.572	-1.716	2.908	1.00	44.18
	ATOM	1878	C	LEU	541	26.723	-3.676	5.833	1.00	39.75
20	ATOM	1879	O	LEU	541	25.616	-3.713	5.297	1.00	36.48
	ATOM	1880	N	GLU	542	27.366	-4.770	6.230	1.00	40.88
	ATOM	1881	CA	GLU	542	26.790	-6.097	6.037	1.00	41.89
	ATOM	1882	CB	GLU	542	27.719	-7.170	6.620	1.00	44.11
	ATOM	1883	CG	GLU	542	27.010	-8.457	7.052	1.00	50.60
25	ATOM	1884	CD	GLU	542	26.434	-9.245	5.887	1.00	55.80
	ATOM	1885	OE1	GLU	542	25.570	-10.117	6.130	1.00	58.81
	ATOM	1886	OE2	GLU	542	26.842	-8.996	4.728	1.00	57.19
	ATOM	1887	C	GLU	542	25.414	-6.195	6.691	1.00	41.58
	ATOM	1888	O	GLU	542	24.472	-6.720	6.102	1.00	42.82
30	ATOM	1889	N	MET	543	25.298	-5.686	7.915	1.00	40.09
	ATOM	1890	CA	MET	543	24.036	-5.731	8.634	1.00	36.43
	ATOM	1891	CB	MET	543	24.270	-5.424	10.111	1.00	39.95
	ATOM	1892	CG	MET	543	25.137	-6.459	10.808	1.00	41.95
	ATOM	1893	SD	MET	543	24.918	-6.445	12.604	1.00	47.17
35	ATOM	1894	CE	MET	543	25.324	-4.749	12.964	1.00	40.88
	ATOM	1895	C	MET	543	23.001	-4.769	8.072	1.00	35.02
	ATOM	1896	O	MET	543	21.808	-5.073	8.048	1.00	35.31
	ATOM	1897	N	LEU	544	23.457	-3.605	7.629	1.00	32.90
	ATOM	1898	CA	LEU	544	22.559	-2.603	7.074	1.00	36.88
40	ATOM	1899	CB	LEU	544	23.225	-1.226	7.111	1.00	34.51
	ATOM	1900	CG	LEU	544	23.268	-0.562	8.490	1.00	31.94
	ATOM	1901	CD1	LEU	544	24.284	0.564	8.478	1.00	32.27
	ATOM	1902	CD2	LEU	544	21.897	-0.029	8.846	1.00	29.02
	ATOM	1903	C	LEU	544	22.148	-2.941	5.640	1.00	38.94
45	ATOM	1904	O	LEU	544	20.971	-2.842	5.294	1.00	39.52
	ATOM	1905	N	ASP	545	23.118	-3.338	4.817	1.00	41.05
	ATOM	1906	CA	ASP	545	22.850	-3.685	3.418	1.00	40.78
	ATOM	1907	CB	ASP	545	24.159	-3.780	2.620	1.00	37.75

ATOM	1908	CG	ASP	545	23.922	-3.937	1.120	1.00	35.19
ATOM	1909	OD1	ASP	545	24.881	-4.265	0.380	1.00	33.48
ATOM	1910	OD2	ASP	545	22.768	-3.734	0.691	1.00	31.33
ATOM	1911	C	ASP	545	22.116	-5.015	3.349	1.00	42.87
ATOM	1912	O	ASP	545	22.681	-6.030	2.929	1.00	44.32
ATOM	1913	N	ALA	546	20.853	-5.009	3.755	1.00	43.49
ATOM	1914	CA	ALA	546	20.069	-6.229	3.746	1.00	46.96
ATOM	1915	CB	ALA	546	19.213	-6.305	5.006	1.00	47.82
ATOM	1916	C	ALA	546	19.193	-6.362	2.508	1.00	49.55
ATOM	1917	O	ALA	546	18.804	-5.368	1.883	1.00	48.75
ATOM	1918	N	HIS	547	18.895	-7.606	2.152	1.00	50.98
ATOM	1919	CA	HIS	547	18.042	-7.884	1.006	1.00	53.77
ATOM	1920	CB	HIS	547	18.431	-9.223	0.369	1.00	52.69
ATOM	1921	CG	HIS	547	18.395	-10.382	1.317	1.00	55.05
ATOM	1922	CD2	HIS	547	17.477	-10.752	2.242	1.00	53.94
ATOM	1923	ND1	HIS	547	19.395	-11.329	1.371	1.00	56.23
ATOM	1924	CE1	HIS	547	19.095	-12.232	2.286	1.00	55.36
ATOM	1925	NE2	HIS	547	17.936	-11.906	2.830	1.00	57.01
ATOM	1926	C	HIS	547	16.603	-7.936	1.518	1.00	55.69
ATOM	1927	O	HIS	547	16.362	-7.796	2.720	1.00	54.30
ATOM	1928	N	ARG	548	15.653	-8.139	0.612	1.00	57.00
ATOM	1929	CA	ARG	548	14.245	-8.212	0.987	1.00	60.65
ATOM	1930	CB	ARG	548	13.432	-7.171	0.208	1.00	62.69
ATOM	1931	CG	ARG	548	14.272	-6.222	-0.637	1.00	67.54
ATOM	1932	CD	ARG	548	13.448	-5.061	-1.171	1.00	71.92
ATOM	1933	NE	ARG	548	13.702	-3.826	-0.432	1.00	76.95
ATOM	1934	CZ	ARG	548	14.864	-3.178	-0.429	1.00	79.04
ATOM	1935	NH1	ARG	548	15.891	-3.644	-1.128	1.00	80.66
ATOM	1936	NH2	ARG	548	15.001	-2.063	0.278	1.00	80.39
ATOM	1937	C	ARG	548	13.695	-9.608	0.711	1.00	61.65
ATOM	1938	O	ARG	548	12.500	-9.781	0.466	1.00	62.05
ATOM	1939	N	LEU	549	14.576	-10.603	0.756	1.00	62.39
ATOM	1940	CA	LEU	549	14.188	-11.985	0.507	1.00	64.02
ATOM	1941	CB	LEU	549	15.433	-12.828	0.195	1.00	62.14
ATOM	1942	CG	LEU	549	16.461	-12.191	-0.753	1.00	60.76
ATOM	1943	CD1	LEU	549	17.699	-13.074	-0.878	1.00	57.77
ATOM	1944	CD2	LEU	549	15.823	-11.972	-2.108	1.00	58.38
ATOM	1945	C	LEU	549	13.431	-12.574	1.702	1.00	66.65
ATOM	1946	O	LEU	549	12.759	-13.600	1.577	1.00	67.15
ATOM	1947	N	HIS	550	13.541	-11.920	2.856	1.00	67.72
ATOM	1948	CA	HIS	550	12.858	-12.378	4.065	1.00	69.93
ATOM	1949	CB	HIS	550	13.753	-12.190	5.298	1.00	70.76
ATOM	1950	CG	HIS	550	14.977	-13.054	5.306	1.00	71.50
ATOM	1951	CD2	HIS	550	15.539	-13.821	4.341	1.00	71.63
ATOM	1952	ND1	HIS	550	15.793	-13.172	6.411	1.00	71.98
ATOM	1953	CE1	HIS	550	16.805	-13.972	6.126	1.00	72.04
ATOM	1954	NE2	HIS	550	16.674	-14.379	4.876	1.00	71.39
ATOM	1955	C	HIS	550	11.556	-11.603	4.275	1.00	71.15

ATOM	1956	O	HIS	550	10.940	-11.684	5.340	1.00	70.66
ATOM	1957	N	ALA	551	11.143	-10.851	3.258	1.00	72.22
ATOM	1958	CA	ALA	551	9.919	-10.057	3.338	1.00	73.58
ATOM	1959	CB	ALA	551	9.904	-9.014	2.221	1.00	73.21
ATOM	1960	C	ALA	551	8.658	-10.920	3.266	1.00	74.69
ATOM	1961	O	ALA	551	7.684	-10.474	2.621	1.00	76.12
ATOM	1962	OXT	ALA	551	8.651	-12.025	3.852	1.00	73.79
HETATM	1963	C10	OHT	600	30.581	1.481	29.471	1.00	26.84
HETATM	1964	C9	OHT	600	30.713	-0.043	29.358	1.00	22.85
HETATM	1965	C8	OHT	600	31.366	-0.385	28.037	1.00	25.56
HETATM	1966	C11	OHT	600	32.761	0.051	27.916	1.00	27.51
HETATM	1967	C16	OHT	600	33.218	0.797	26.797	1.00	28.35
HETATM	1968	C15	OHT	600	34.551	1.237	26.747	1.00	30.39
HETATM	1969	C14	OHT	600	35.443	0.923	27.792	1.00	30.23
HETATM	1970	C13	OHT	600	35.004	0.185	28.890	1.00	31.45
HETATM	1971	C12	OHT	600	33.666	-0.241	28.955	1.00	27.93
HETATM	1972	C7	OHT	600	30.682	-1.089	27.077	1.00	24.41
HETATM	1973	C1	OHT	600	29.211	-1.258	27.052	1.00	24.26
HETATM	1974	C2	OHT	600	28.644	-2.526	26.706	1.00	25.92
HETATM	1975	C3	OHT	600	27.254	-2.668	26.580	1.00	26.32
HETATM	1976	C4	OHT	600	26.438	-1.553	26.813	1.00	29.02
HETATM	1977	O4	OHT	600	25.072	-1.605	26.716	1.00	28.42
HETATM	1978	C5	OHT	600	26.980	-0.286	27.130	1.00	26.98
HETATM	1979	C6	OHT	600	28.362	-0.147	27.231	1.00	25.23
HETATM	1980	C17	OHT	600	31.370	-1.692	25.942	1.00	26.61
HETATM	1981	C18	OHT	600	32.508	-2.498	26.151	1.00	26.77
HETATM	1982	C19	OHT	600	33.166	-3.052	25.072	1.00	27.50
HETATM	1983	C20	OHT	600	32.676	-2.794	23.786	1.00	27.50
HETATM	1984	O20	OHT	600	33.206	-3.566	22.795	1.00	31.35
HETATM	1985	C23	OHT	600	33.009	-3.135	21.448	1.00	40.09
HETATM	1986	C24	OHT	600	34.226	-3.490	20.575	1.00	44.80
HETATM	1987	N24	OHT	600	34.141	-4.901	20.203	1.00	49.00
HETATM	1988	C25	OHT	600	33.375	-5.040	18.933	1.00	51.64
HETATM	1989	C26	OHT	600	35.495	-5.459	20.004	1.00	52.06
HETATM	1990	C21	OHT	600	31.540	-2.005	23.558	1.00	27.19
HETATM	1991	C22	OHT	600	30.892	-1.450	24.645	1.00	27.92
HETATM	1992	O1	HOH	1	20.714	-12.010	23.057	1.00	27.20
HETATM	1993	O1	HOH	2	22.563	-0.070	25.819	1.00	25.77
HETATM	1994	O1	HOH	3	25.183	19.202	23.149	1.00	42.52
HETATM	1995	O1	HOH	4	35.158	5.823	37.390	1.00	33.92
HETATM	1996	O1	HOH	5	22.116	-9.922	18.914	1.00	30.18
HETATM	1997	O1	HOH	6	29.812	6.536	19.652	1.00	26.11
HETATM	1998	O1	HOH	7	13.362	4.463	20.376	1.00	29.40
HETATM	1999	O1	HOH	8	19.799	-11.295	20.187	1.00	28.70
HETATM	2000	O1	HOH	9	21.205	1.466	23.794	1.00	22.47
HETATM	2001	O1	HOH	10	21.177	-4.961	29.066	1.00	33.00
HETATM	2002	O1	HOH	11	18.591	1.863	20.518	1.00	32.59
HETATM	2003	O1	HOH	12	16.298	21.566	15.992	1.00	33.42

	HETATM 2004	O1	HOH	13	18.611	1.976	24.494	1.00	29.70
	HETATM 2005	O1	HOH	14	38.009	8.910	21.156	1.00	39.92
	HETATM 2006	O1	HOH	15	26.549	11.664	18.080	1.00	30.25
	HETATM 2007	O1	HOH	16	20.282	-4.239	26.512	1.00	32.70
5	HETATM 2008	O1	HOH	17	32.858	8.754	20.237	1.00	29.88
	HETATM 2009	O1	HOH	18	8.497	16.136	29.934	1.00	46.80
	HETATM 2010	O1	HOH	19	21.940	19.301	31.632	1.00	35.72
	HETATM 2011	O1	HOH	20	35.153	2.682	14.122	1.00	41.02
	HETATM 2012	O1	HOH	21	20.358	-2.268	21.013	1.00	29.43
10	HETATM 2013	O1	HOH	22	35.562	10.036	36.334	1.00	41.37
	HETATM 2014	O1	HOH	23	17.248	18.187	17.571	1.00	33.96
	HETATM 2015	O1	HOH	24	18.445	20.973	12.346	1.00	43.44
	HETATM 2016	O1	HOH	25	12.152	23.054	33.132	1.00	36.04
	HETATM 2017	O1	HOH	26	13.181	22.222	9.699	1.00	37.03
15	HETATM 2018	O1	HOH	27	19.399	-6.090	12.808	1.00	44.86
	HETATM 2019	O1	HOH	28	37.895	13.599	31.395	1.00	47.26
	HETATM 2020	O1	HOH	29	11.570	6.212	7.962	1.00	51.10
	HETATM 2021	O1	HOH	30	20.172	-2.568	23.445	1.00	51.70
	HETATM 2022	O1	HOH	31	36.402	-5.369	23.729	1.00	58.20
20	HETATM 2023	O1	HOH	32	25.127	13.802	19.187	1.00	35.29
	HETATM 2024	O1	HOH	33	23.181	4.937	38.538	1.00	33.77
	HETATM 2025	O1	HOH	34	20.550	0.421	21.276	1.00	29.12
	HETATM 2026	O1	HOH	35	39.599	13.954	27.312	1.00	44.08
	HETATM 2027	O1	HOH	36	26.445	13.863	21.285	1.00	34.97
25	HETATM 2028	O1	HOH	37	13.759	5.079	9.108	1.00	38.54
	HETATM 2029	O1	HOH	38	14.150	24.731	34.529	1.00	49.72
	HETATM 2030	O1	HOH	39	21.060	13.886	-6.319	1.00	59.79
	HETATM 2031	O1	HOH	40	32.215	6.217	8.726	1.00	60.22
	HETATM 2032	O1	HOH	41	35.105	15.704	9.069	1.00	45.15
30	HETATM 2033	O1	HOH	42	11.427	19.451	9.903	1.00	38.56
	HETATM 2034	O1	HOH	43	19.662	23.472	10.333	1.00	47.71
	HETATM 2035	O1	HOH	44	9.231	3.690	12.337	1.00	45.98
	HETATM 2036	O1	HOH	45	15.313	-6.036	17.192	1.00	39.07
	HETATM 2037	O1	HOH	46	15.517	-3.266	17.907	1.00	37.67
35	HETATM 2038	O1	HOH	47	28.784	-16.713	25.163	1.00	55.44
	HETATM 2039	O1	HOH	48	27.868	-10.898	28.271	1.00	31.27
	HETATM 2040	O1	HOH	49	6.955	13.568	28.233	1.00	48.83
	HETATM 2041	O1	HOH	50	22.051	-15.030	28.603	1.00	36.91
	HETATM 2042	O1	HOH	51	7.026	31.002	30.284	1.00	46.73
40	HETATM 2043	O1	HOH	52	-1.489	12.385	15.164	1.00	51.17
	HETATM 2044	O1	HOH	53	3.499	6.444	14.452	1.00	50.38
	HETATM 2045	O1	HOH	54	18.655	-2.048	25.518	1.00	52.29
	HETATM 2046	O1	HOH	55	28.188	-15.195	38.996	1.00	55.22
	HETATM 2047	O1	HOH	56	35.275	-10.556	38.061	1.00	57.39
45	HETATM 2048	O1	HOH	57	37.771	-9.103	34.605	1.00	54.17
	HETATM 2049	O1	HOH	58	31.403	-3.039	17.983	1.00	46.80
	HETATM 2050	O1	HOH	59	30.455	-6.352	17.005	1.00	47.05
	HETATM 2051	O1	HOH	60	25.985	8.255	0.416	1.00	43.32

HETATM 2052	O1	HOH	61	35.679	0.749	10.462	1.00	42.99
HETATM 2053	O1	HOH	62	14.741	4.029	33.936	1.00	49.59
HETATM 2054	O1	HOH	63	16.333	2.592	35.952	1.00	45.13
HETATM 2055	O1	HOH	64	23.809	7.186	39.798	1.00	45.36
HETATM 2056	O1	HOH	65	27.012	-1.948	46.995	1.00	63.39
HETATM 2057	O1	HOH	66	25.956	-6.422	42.144	1.00	44.94
HETATM 2058	O1	HOH	67	23.510	-8.414	39.036	1.00	39.06
HETATM 2059	O1	HOH	68	41.475	0.971	33.110	1.00	55.50
HETATM 2060	O1	HOH	69	36.519	8.863	38.836	1.00	41.56
HETATM 2061	O1	HOH	70	30.111	14.823	12.793	1.00	44.58
HETATM 2062	O1	HOH	71	26.850	-6.092	1.594	1.00	40.15
HETATM 2063	O1	HOH	72	20.448	-3.169	1.055	1.00	42.50
HETATM 2064	O1	HOH	73	33.896	3.047	16.172	1.00	46.39
HETATM 2065	O1	HOH	74	16.884	0.446	26.043	1.00	61.50
HETATM 2066	O1	HOH	75	18.595	0.296	27.866	1.00	47.33
HETATM 2067	O1	HOH	76	6.166	21.439	19.124	1.00	47.94
HETATM 2068	O1	HOH	77	18.484	20.060	16.232	1.00	35.52
HETATM 2069	O1	HOH	78	1.985	23.265	29.187	1.00	46.42
HETATM 2070	O1	HOH	79	12.729	30.461	27.530	1.00	62.79
END								

CLAIMS

WHAT IS CLAIMED IS:

1. A method of identifying a compound that modulates nuclear receptor activity, said method comprising:

modeling test compounds that fit spatially into a nuclear receptor ligand binding domain of interest using an atomic structural model of the estrogen receptor α ligand binding domain or portion thereof,

screening said test compounds in an assay characterized by binding of a test compound to the ligand binding domain, and

identifying a test compound that modulates nuclear receptor activity, wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human estrogen receptor α Met343, Leu346, Ala350, Glu353, Leu384, Leu387, Leu391, Arg394, Phe404, Met421, Leu428, Gly521, His524, Leu525 and Met528.

2. The method of Claim 1 wherein the amino acid residues correspond to residues Met343, Met421, His524, Leu525 and Met528.

3. The method of Claim 1 wherein the test compound is an agonist and nuclear receptor activity is measured by binding of a coactivator to the coactivator binding site.

4. The method of Claim 1 wherein the test compound is an antagonist and nuclear receptor activity is measured by the unwinding of helix 12.

5. The method of Claim 1 wherein the test compound is an antagonist and nuclear receptor activity is measured by the blocking of coactivator binding.

6. The method of Claim 1 wherein said screening is *in vitro*.

7. The method of Claim 6 wherein said screening is high throughput screening.

8. The method of Claim 1 wherein said test compound is from a library of compounds.

9. The method of Claim 1 wherein said test compound is a small organic molecule, a peptide, or peptidomimetic.

10. The method of Claim 1 which further comprises the step of providing the atomic coordinates of the estrogen receptor α ligand binding domain or portion thereof to a computerized modeling system, prior to said modeling step.

11. The method of Claim 1 wherein said nuclear receptor is selected from the group consisting of estrogen receptors, thyroid receptors, retinoid receptors, glucocorticoid receptors,

progestin receptors, mineralocorticoid receptors, androgen receptors, peroxisome receptors and vitamin D receptors.

12. The method of Claim 11 wherein said nuclear receptor is an estrogen receptor.

13. The method of Claim 12 wherein said estrogen receptor is the estrogen receptor α.

14. A method of identifying a compound that modulates ligand binding to a nuclear receptor, said method comprising:

modeling test compounds that fit spacially into a nuclear receptor ligand binding domain of interest using an atomic structural model of the estrogen receptor α ligand binding domain or portion thereof,

screening said test compounds in an assay characterized by binding of a test compound to the binding domain, and

identifying a test compound that modulates ligand binding to said nuclear receptor,

wherein said atomic structural model comprises atomic coordinates of amino acid residues corresponding to residues of human estrogen receptor α Met343, Leu346, Ala350, Glu353, Leu384, Leu387, Leu391, Arg394, Phe404, Met421, Leu428, Gly521, His524, Leu525 and Met528.

15. The method of Claim 14 wherein the amino acid residues correspond to residues Met343, Met421, His524, Leu525 and Met528.

16. The method of Claim 14 wherein said nuclear receptor is selected from the group consisting of estrogen receptors, thyroid receptors, retinoid receptors, glucocorticoid receptors, progestin receptors, mineralocorticoid receptors, androgen receptors, peroxisome receptors and vitamin D receptors.

17. The method of Claim 16 wherein said nuclear receptor is an estrogen receptor.

18. The method of Claim 17 wherein said estrogen receptor is the estrogen receptor α.

19. The method of Claim 14 wherein said screening is *in vitro*.

20. The method of Claim 19 wherein said screening is high throughput screening.

21. The method of Claim 14 wherein said test compound is from a library of compounds.

22. The method of Claim 14 wherein said test compound is an agonist or antagonist of ligand binding.

23. The method of Claim 14 wherein said test compound is a small organic molecule, a peptide, or peptidomimetic.

24. A method for identifying an agonist or antagonist of ligand binding to a nuclear receptor, said method comprising the steps of:

providing the atomic coordinates of the estrogen receptor α ligand binding domain or portion thereof to a computerized modeling system, wherein said atomic coordinates are of the amino acid residues corresponding to residues of human estrogen receptor α Met343, Leu346, Ala350, Glu353, Leu384, Leu387, Leu391, Arg394, Phe404, Met421, Leu428, Gly521, His524, Leu525 and Met528;

modeling compounds which fit spacially into the ligand binding domain; and

identifying in an assay for nuclear receptor activity a compound which increases or decreases the activity of the nuclear receptor by binding the ligand binding domain of said nuclear receptor, whereby an agonist or antagonist of ligand binding is identified.

25. The method of Claim 24 wherein the amino acid residues correspond to residues Met343, Met421, His524, Leu525 and Met528.

26. The method of Claim 24 wherein said nuclear receptor is selected from the group consisting of estrogen receptors, thyroid receptors, retinoid receptors, glucocorticoid receptors, progestin receptors, mineralocorticoid receptors, androgen receptors, peroxisome receptors and vitamin D receptors.

27. The method of Claim 26 wherein said nuclear receptor is an estrogen receptor.

28. The method of Claim 27 wherein said estrogen receptor is the estrogen receptor α.

29. A method of modulating nuclear receptor activity in a mammal by administering to a mammal in need thereof a sufficient amount of a compound that fits spatially and preferentially into a ligand binding domain of a nuclear receptor of interest, where said compound is designed so as to distort at least one amino acid residue corresponding to residues of human estrogen receptor α Met343, Leu346, Ala350, Glu353, Leu384, Leu387, Leu391, Arg394, Phe404, Met421, Leu428, Gly521, His524, Leu525 and Met528.

30. The method of Claim 29 wherein at least one amino acid residue corresponds to residues Met343, Met421, His524, Leu525 and Met528.

31. The method of Claim 29 wherein said nuclear receptor is selected from the group consisting of estrogen receptors, thyroid receptors, retinoid receptors, glucocorticoid receptors, progestin receptors, mineralocorticoid receptors, androgen receptors, peroxisome receptors and vitamin D receptors.

32. The method of Claim 31 wherein said nuclear receptor is an estrogen receptor.

33. The method of Claim 32 wherein said estrogen receptor is the estrogen receptor α.

34. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecular complex of a compound bound to a nuclear receptor ligand binding domain comprising structure coordinates of amino acids corresponding to human estrogen receptor α Met343, Leu346, Ala350, Glu353, Leu384, Leu387, Leu391, Arg394, Phe404, Met421, Leu428, Gly521, His524, Leu525 and Met528 or a homologue of said molecular complex, wherein said homologue comprises a ligand binding domain that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

35. The machine-readable data storage medium of Claim 34 wherein the amino acid residues correspond to residues Met343, Met421, His524, Leu525 and Met528.

36. The machine-readable data storage medium of Claim 34 wherein said nuclear receptor is selected from the group consisting of estrogen receptors, thyroid receptors, retinoid receptors, glucocorticoid receptors, progestin receptors, mineralocorticoid receptors, androgen receptors, peroxisome receptors and vitamin D receptors.

37. The machine-readable data storage medium of Claim 36 wherein said nuclear receptor is an estrogen receptor.

38. The machine-readable data storage medium of Claim 37 wherein said estrogen receptor is the estrogen receptor α.

39. The machine-readable data storage medium of Claim 34 wherein said molecular complex is defined by the set of structure coordinates depicted in Appendix 1 or Appendix 2, or a homologue of said molecular complex, said homologue having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

40. A machine-readable data storage medium comprising a data storage material encoded with a first set of machine readable data which, when combined with a second set of machine readable data, using a machine programmed with instructions for using said first set of data and said second set of data, can determine at least a portion of the structure coordinates corresponding to the second set of machine readable data, wherein: said first set of data comprises a Fourier transform of at least a portion of the structural coordinates selected from the group consisting of coordinates depicted in Appendix 1 or Appendix 2; and said

second set of data comprises an X-ray diffraction pattern of a molecule or molecular complex.

41. The machine-readable data storage medium of Claim 40 wherein said nuclear receptor is selected from the group consisting of estrogen receptors, thyroid receptors, retinoid receptors, glucocorticoid receptors, progestin receptors, mineralocorticoid receptors, androgen receptors, peroxisome receptors and vitamin D receptors.

42. The machine-readable data storage medium of Claim 41 wherein said nuclear receptor is an estrogen receptor.

43. The machine-readable data storage medium of Claim 42 wherein said estrogen receptor is the estrogen receptor α.

44. A cocrystal of a nuclear receptor comprising an agonist bound to the ligand binding domain and a molecule bound to the coactivator binding site of the nuclear receptor, wherein said crystal defracts with at least 2.03Å resolution.

45. The cocrystal of Claim 44 wherein said nuclear receptor is the estrogen receptor α.

46. The cocrystal of Claim 45 wherein said estrogen receptor α is human.

47. The cocrystal of Claim 46 wherein said molecule is peptide.

48. The cocrystal of Claim 47 wherein said peptide comprises a NR-box amino acid sequence or derivative thereof.

49. A cocrystal of a nuclear receptor comprising an antagonist bound to the ligand binding domain of the nuclear receptor, wherein said crystal defracts with at least 1.9Å resolution.

50. The cocrystal of Claim 49 wherein said nuclear receptor is the estrogen receptor α.

51. The cocrystal of Claim 50 wherein said estrogen receptor α is human.

52. A computational method of designing a nuclear receptor ligand where at least one amino acid residue of a nuclear receptor LBD that corresponds to human estrogen receptor α Met343, Leu346, Ala350, Glu353, Leu384, Leu387, Leu391, Arg394, Phe404, Met421, Leu428, Gly521, His524, Leu525 and Met528, interacts with at least one first chemical moiety of said ligand, comprising the step of selecting at least one chemical modification of said first chemical moiety to produce a second chemical moiety with a structure to either decrease or increase an interaction between said interacting amino acid and said second chemical moiety compared to said interaction between said interacting amino acid and said first chemical moiety.

53. The method of Claim 52 wherein at least one amino acid residue corresponds to residues Met343, Met421, His524, Leu525 and Met528.

54. The method of Claim 52 further comprising determining a change in interaction between said interacting amino acid and said ligand after chemical modification of said first chemical moiety.

55. The method of Claim 52 wherein said chemical modification enhances hydrogen bonding interaction, charge interaction, hydrophobic interaction, Van Der Waals interaction or dipole interaction between said second chemical moiety and said interacting amino acid compared to said first chemical moiety and said interacting amino acid.

56. The method of Claim 52 wherein said chemical modification reduces hydrogen bonding interaction, charge interaction, hydrophobic interaction, Van Der Waals interaction or dipole interaction between said second chemical moiety and said interacting amino acid compared to said first chemical moiety and said interacting amino acid.

57. The method of Claim 52 wherein said nuclear receptor is selected from the group consisting of estrogen receptors, thyroid receptors, retinoid receptors, glucocorticoid receptors, progestin receptors, mineralocorticoid receptors, androgen receptors, peroxisome receptors and vitamin D receptors.

58. The method of Claim 57 wherein said nuclear receptor is an estrogen receptor.

59. The method of Claim 52 wherein the estrogen receptor is the estrogen receptor α.

60. The method of Claim 59 wherein the ligand is an agonist.

61. The method of Claim 60 wherein the ligand is selected from the group consisting of 17β-estradiol, diethylstilbestrol, moxestrol, mesohexestrol, coumestrol, Δ^9-THC, o,p-DDT, zearalenone and kepone.

62. The method of Claim 61 wherein the ligand is 17β-estradiol, and the first chemical moiety is a free carbon of the A' ring located at a position selected from the group consisting of C6α, C7α, C12α, C15α, C16α and C17α.

63. The method of Claim 59 wherein the ligand is an antagonist.

64. The method of Claim 63 wherein the ligand is selected from the group consisting of ICI 164,384 and EM800.

65. The method of Claim 59 wherein the ligand is a selective estrogen receptor modulator.

66. The method of Claim 65 wherein the ligand is selected from the group consisting of tamoxifen, raloxifene and GW5638.

67. A method of modulating nuclear receptor activity in a mammal by administering to a mammal in need thereof a sufficient amount of a ligand that fits spatially and preferentially into a ligand binding domain of a nuclear receptor of interest, wherein said ligand is designed by a computational method where at least one amino acid residue of a nuclear receptor ligand binding domain that corresponds to human estrogen receptor α Met343, Leu346, Ala350, Glu353, Leu384, Leu387, Leu391, Arg394, Phe404, Met421, Leu428, Gly521, His524, Leu525 and Met528, interacts with at least one first chemical moiety of said ligand, comprising the step of selecting at least one chemical modification of said first chemical moiety to produce a second chemical moiety with a structure to either decrease or increase an interaction between said interacting amino acid and said second chemical moiety compared to said interaction between said interacting amino acid and said first chemical moiety.

68. The method of Claim 67 wherein at least one amino acid residue corresponds to residues Met343, Met421, His524, Leu525 and Met528.

69. The method of Claim 67 wherein said ligand is an antagonist.

70. The method of Claim 67 wherein said ligand is an agonist.

71. The method of Claim 70 which further comprises administering a coactivator mimic designed by a computational method where at least one amino acid residue of a nuclear receptor coactivator binding site that corresponds to human estrogen receptor α helix 3 residues Leu354, Val355, Met357, Ile358, Ala361 and Lys362, helix 4 residue Phe367, helix 5 residues Gln375, Val376, Leu379 and Glu380, helix 6 residue Trp383, and helix 12 residues Asp538, Leu539, Glu542, Met543 and Leu544, interacts with at least one first chemical moiety of said coactivator mimic, comprising the step of selecting at least one chemical modification of said first chemical moiety to produce a second chemical moiety with a structure to either decrease or increase an interaction between said interacting amino acid and said second chemical moiety compared to said interaction between said interacting amino acid and said first chemical moiety.

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(71) Applicants *(for all designated States except US)*: THE REGENTS OF THE UNIVERSITY OF CALIFORNIA [US/US]; 12th floor, 1111 Franklin Street, Oakland, CA 94607–5200 (US). ARCH DEVELOPMENT CORPORATION [US/US]; 5640 South Ellis Avenue, Chicago, IL 60637 (US).

(72) Inventors; and

(75) Inventors/Applicants *(for US only)*: SHIAU, Andrew [US/US]; Apartment #13, 34 Hugo Street, San Francisco, CA 94122 (US). KUSHNER, Peter, J. [US/US]; 1362 6th Avenue; San Francisco, CA 94122 (US). AGARD, David, A. [US/US]; 238 Juanita Way, San Francisco, CA 94127 (US). GREENE, Geoffrey, L. [US/US]; Apartment 25F, 2020 Lincoln Park West, Chicago, IL 60614 (US).

(74) Agents: EBERLE, Shelley, P.; Cooley Godward LLP, Five Palo Alto Square, 3000 El Camino Real, Palo Alto, CA 94306–2155 (US) et al.

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(57) Abstract

The present invention relates to methods and agonist/antagonist compounds for modulating nuclear receptor activity, and nuclear receptor ligand binding. The invention includes a method for identifying residues comprising a ligand binding domain for a nuclear receptor of interest. Also included in a method of identifying agonists and/or antagonists that bind to the ligand binding domain of the nuclear receptors, and the estrogen receptor in particular. The invention is exemplified by identification and manipulation of the ligand binding domain of the estrogen receptor and compounds that bind to this site. The methods can be applied to other nuclear receptors including TR, GR and PR.

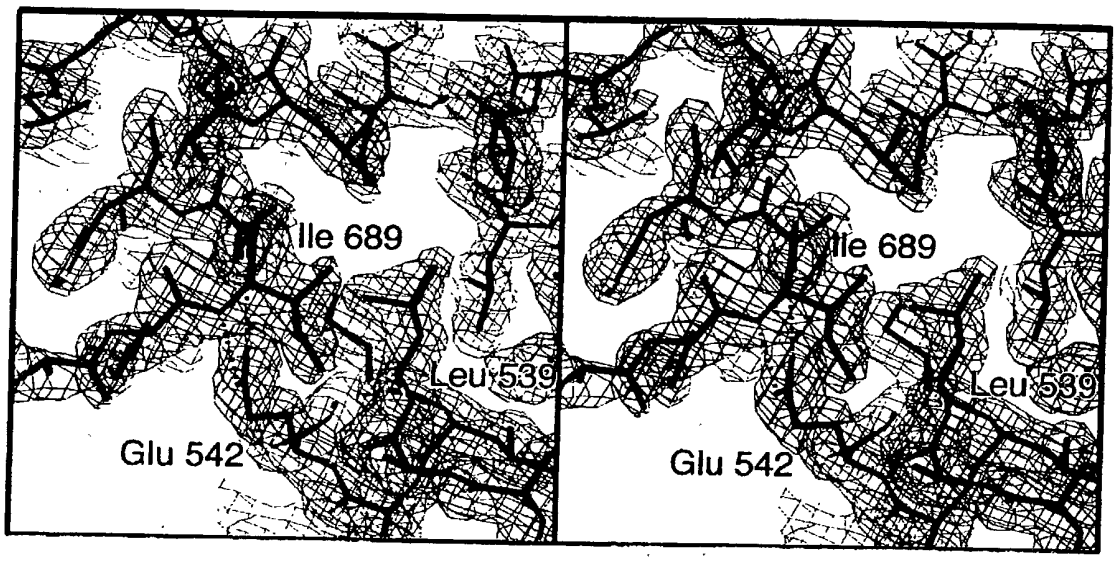
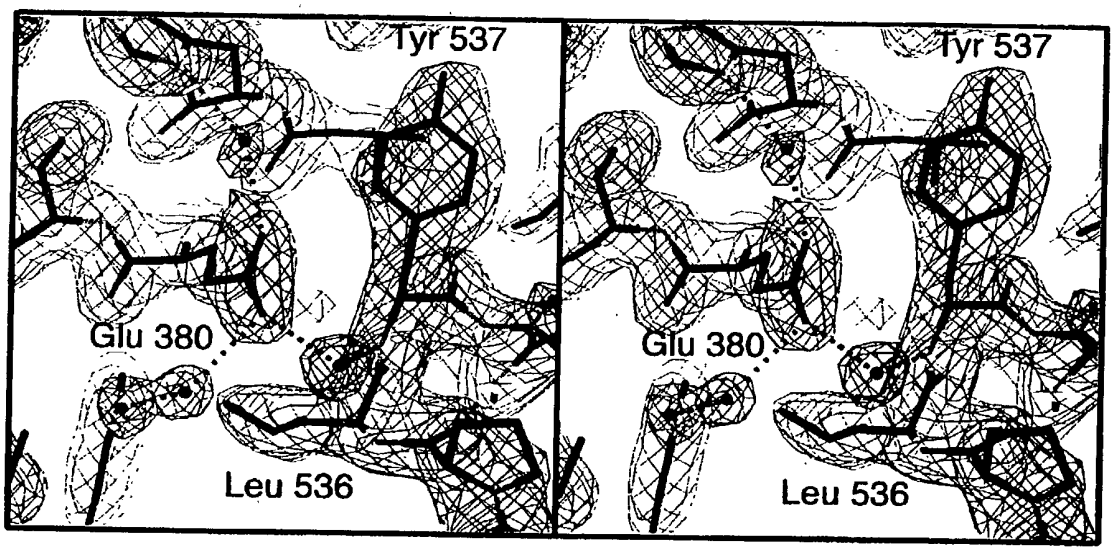

Ile 689
Leu 539
Glu 542
Ile 689
Leu 539
Glu 542

FIG._1A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Glu 380
Leu 536
Tyr 537
Glu 380
Leu 536

FIG._1B

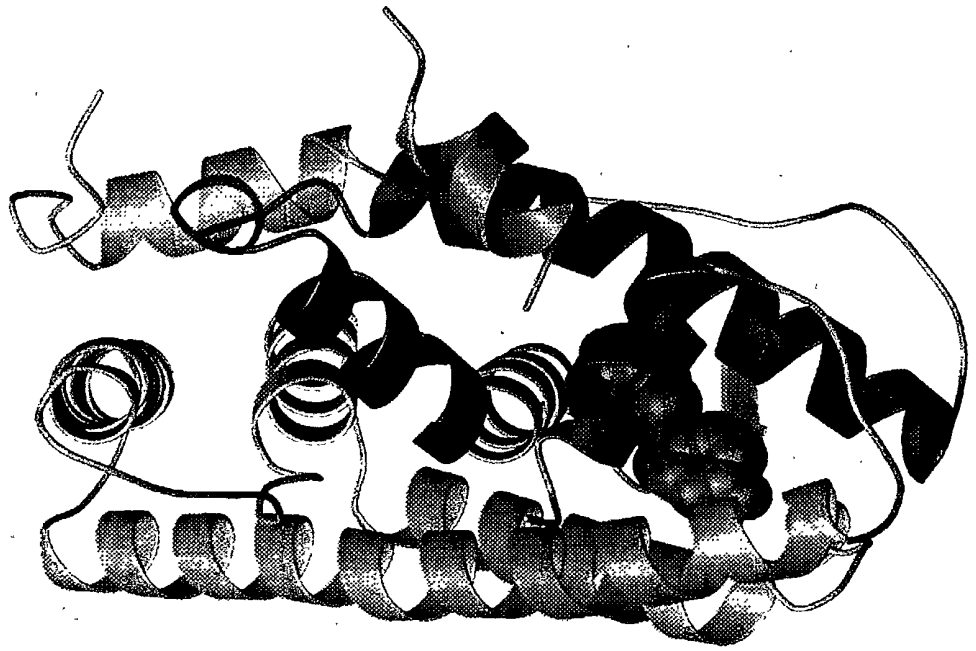


FIG._2A-2

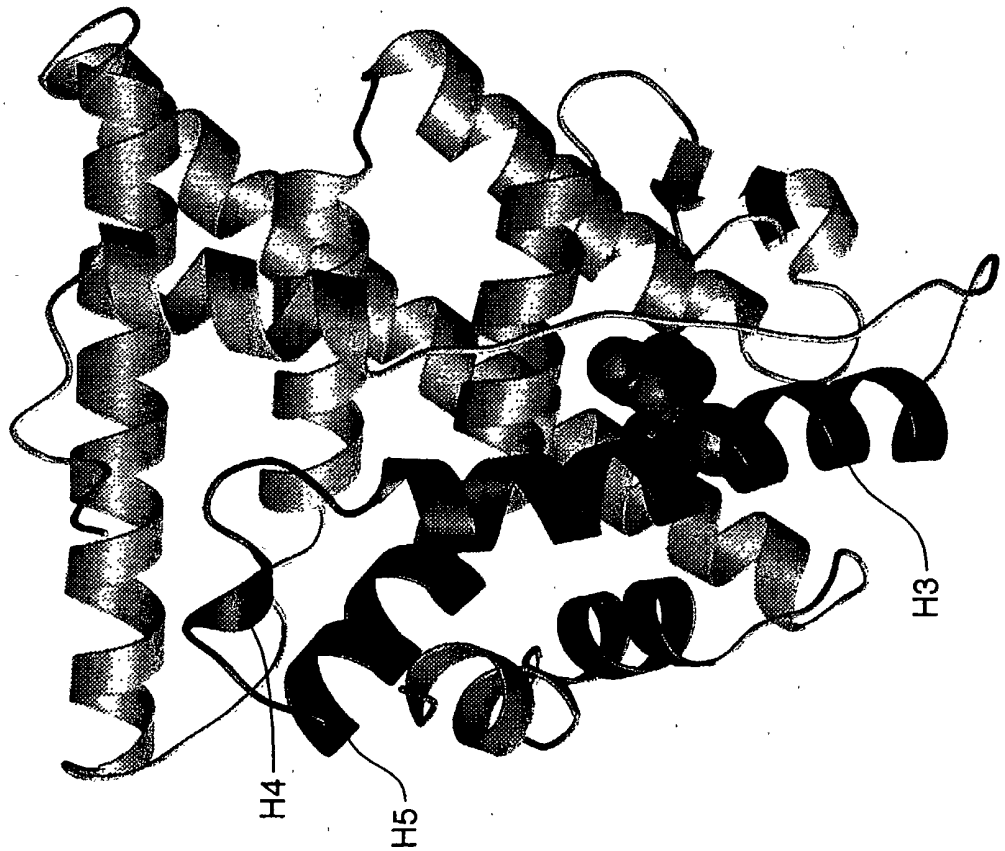


FIG._2A-1

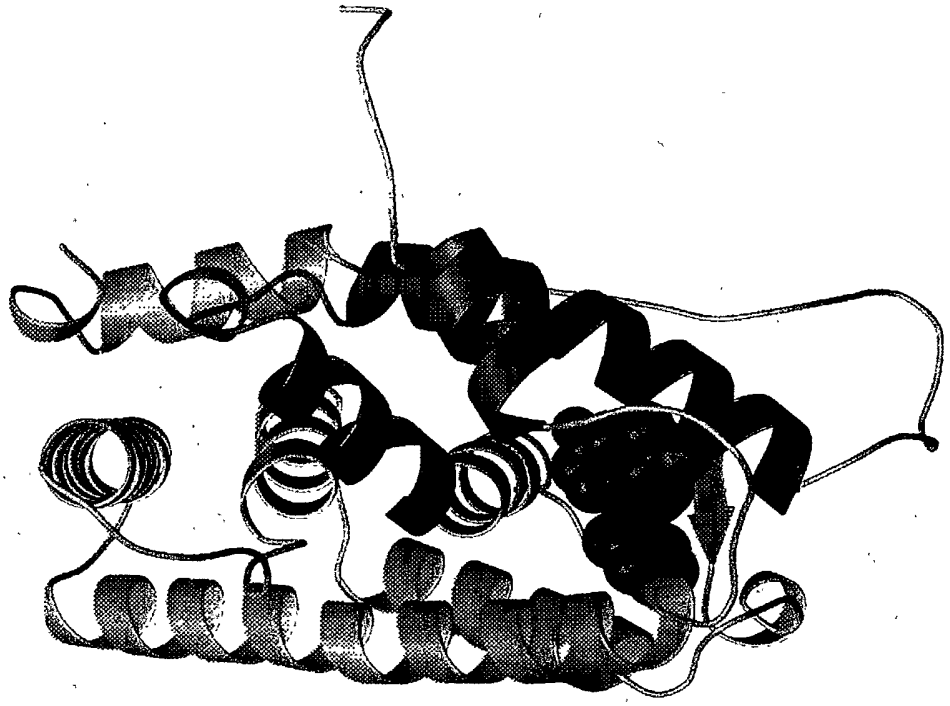


FIG._2B-2

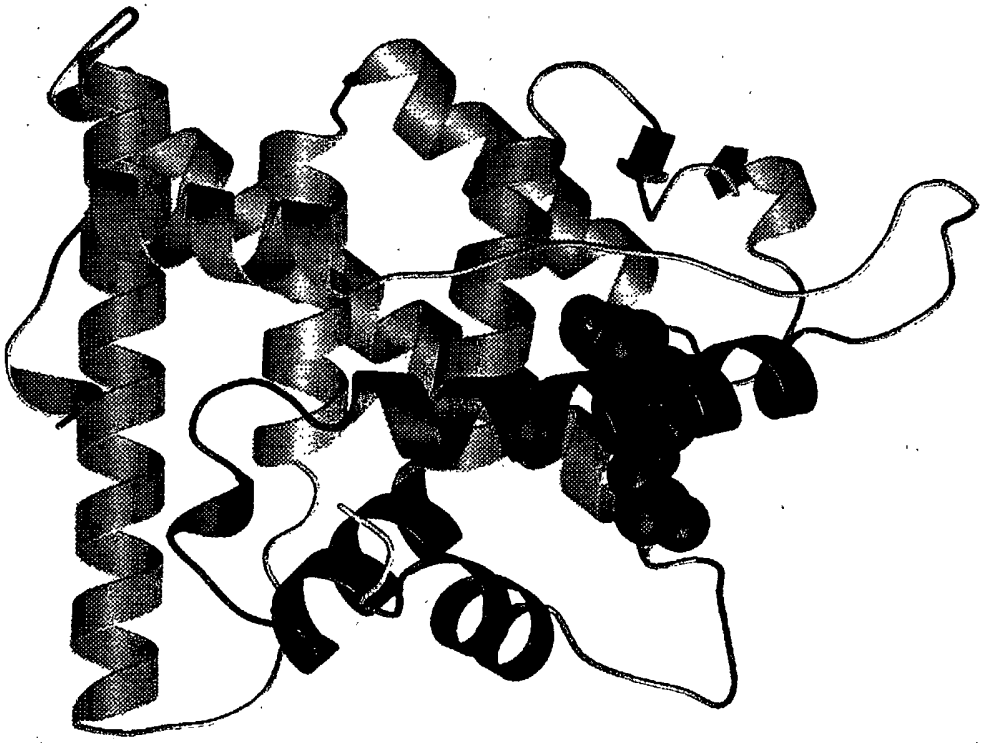


FIG._2B-1

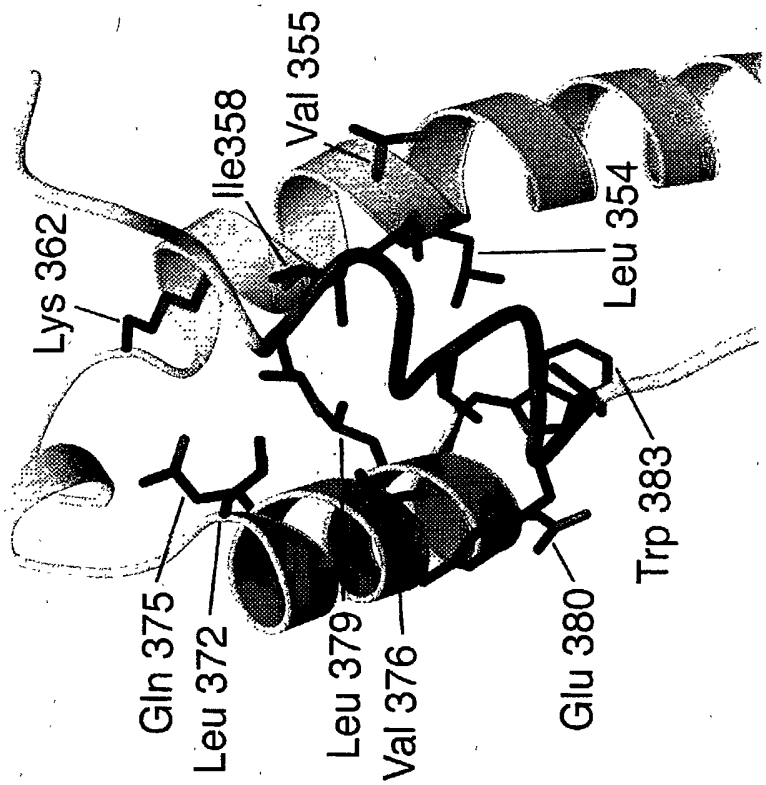

Lys 362
Ile358
Val 355
Leu 354
Gln 375
Leu 372
Leu 379
Val 376
Glu 380
Trp 383

FIG._3B

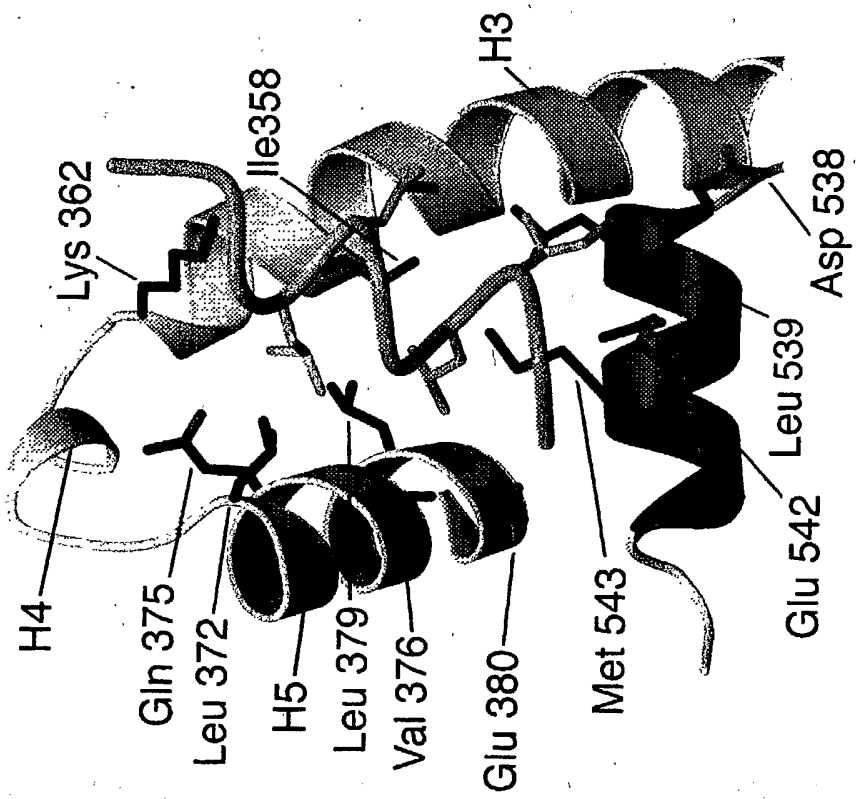

H3
Lys 362
Ile358
Asp 538
Leu 539
H4
Gln 375
Leu 372
H5
Leu 379
Val 376
Glu 380
Met 543
Glu 542

FIG._3A

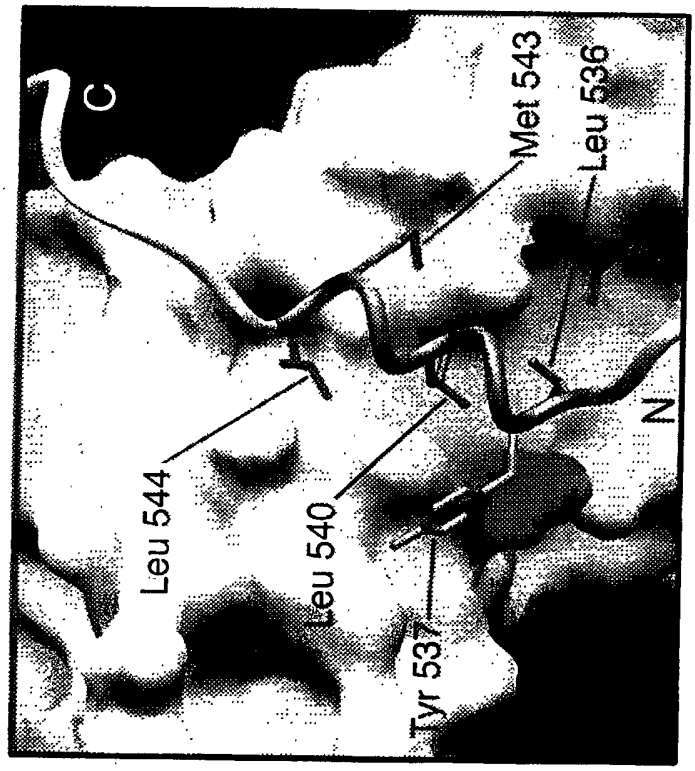

C
Met 543
Leu 536
Leu 544
Leu 540
Tyr 537
N

FIG._3D

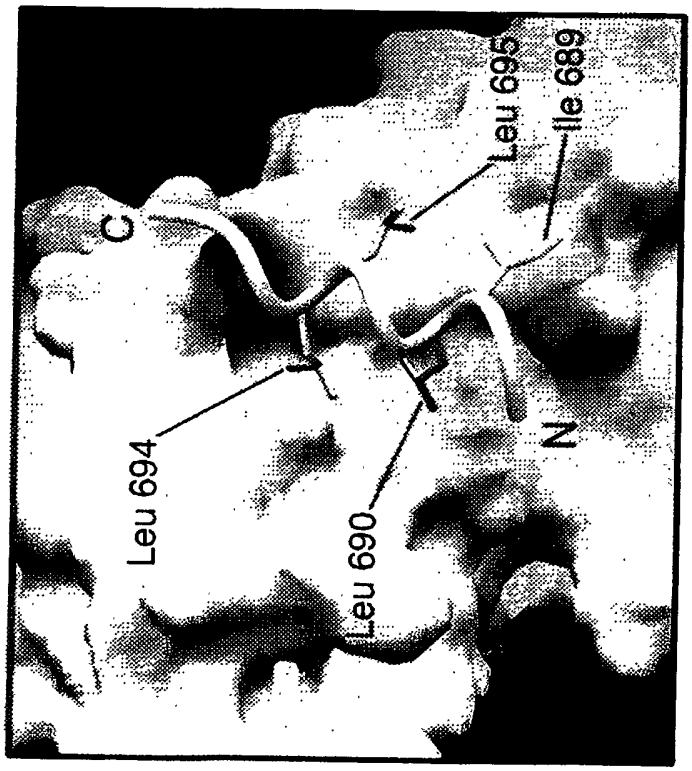

C
Leu 695
Ile 689
Leu 694
Leu 690
N

FIG._3C

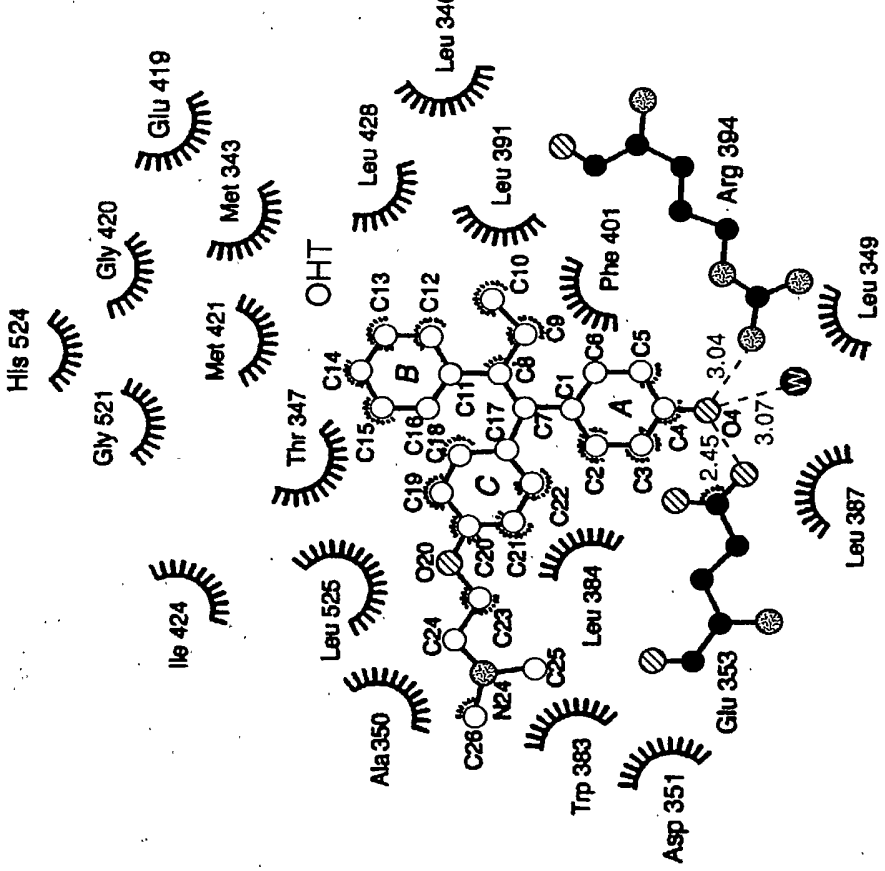

OHT
His 524
Gly 420
Glu 419
Met 343
Leu 346
Leu 428
Leu 391
Phe 401
Arg 394
Leu 349
Gly 521
Met 421
Thr 347
Leu 387
Ile 424
Leu 525
Leu 384
Ala 350
Trp 383
Asp 351
Glu 353
A
B
C
2.45
3.04
3.07

FIG._4B

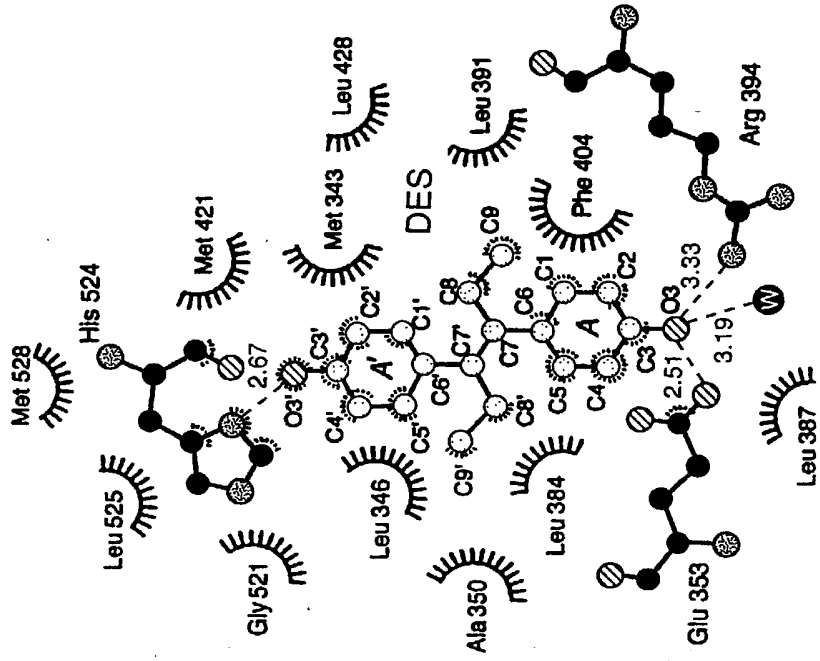

DES
Met 528
His 524
Met 421
Met 343
Leu 428
Leu 391
Phe 404
Arg 394
Leu 525
Gly 521
Leu 346
Ala 350
Leu 384
Glu 353
Leu 387
A
A'
2.67
2.51
3.33
3.19

FIG._4A

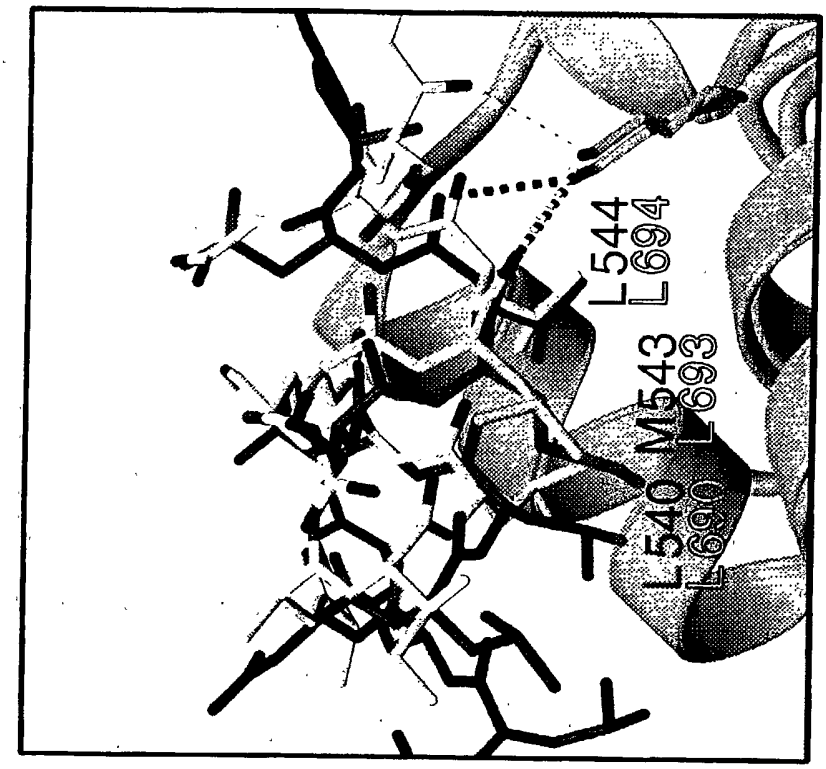


FIG._5B

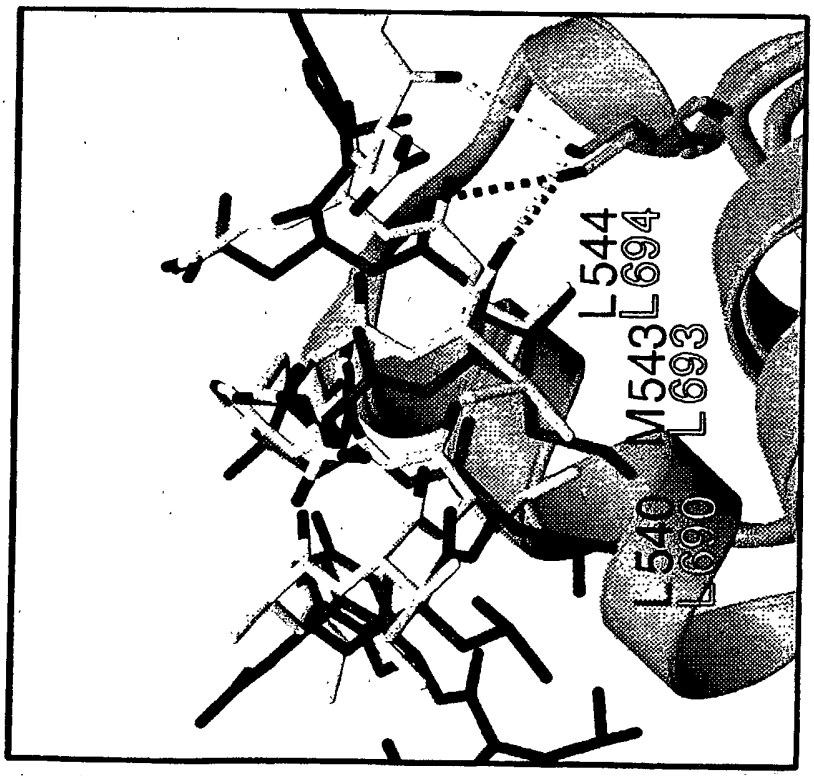


FIG._5A

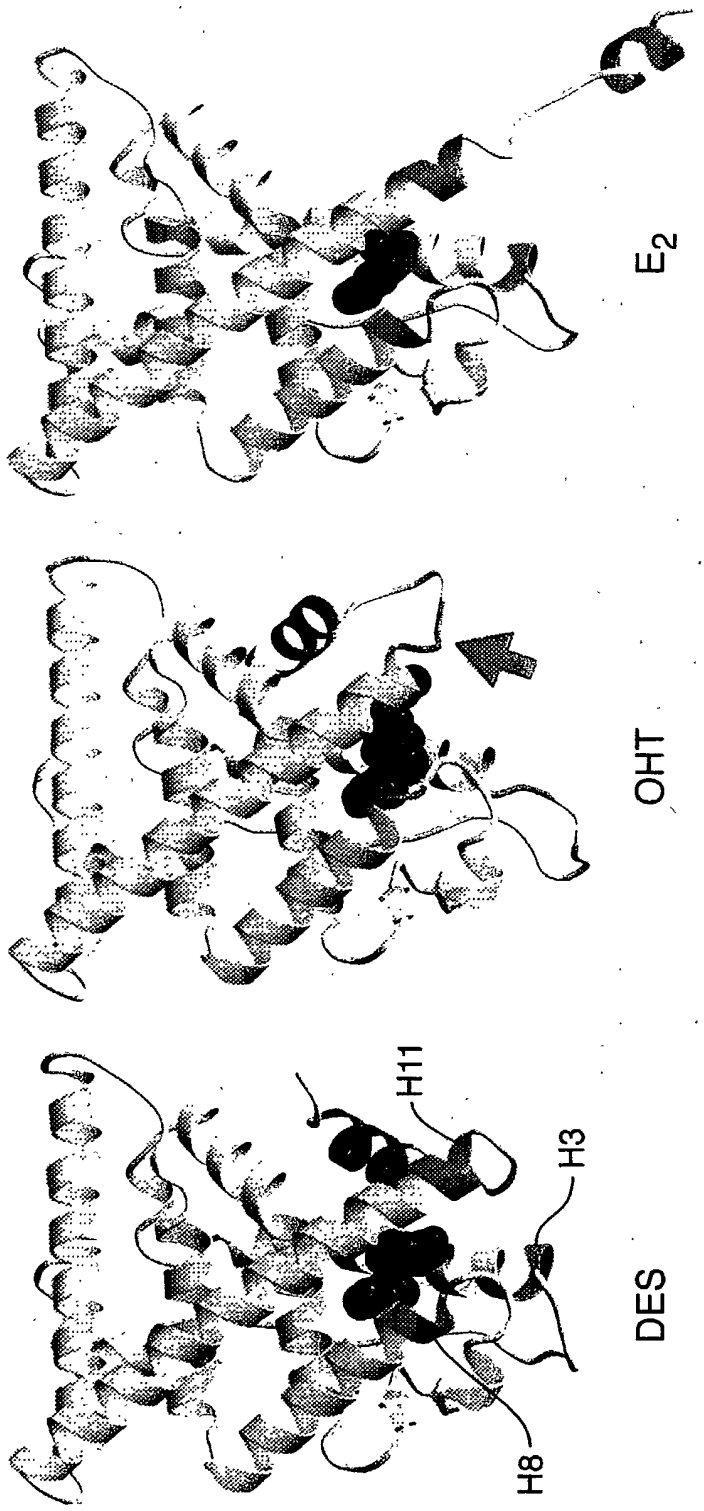


FIG._6A

FIG._6B

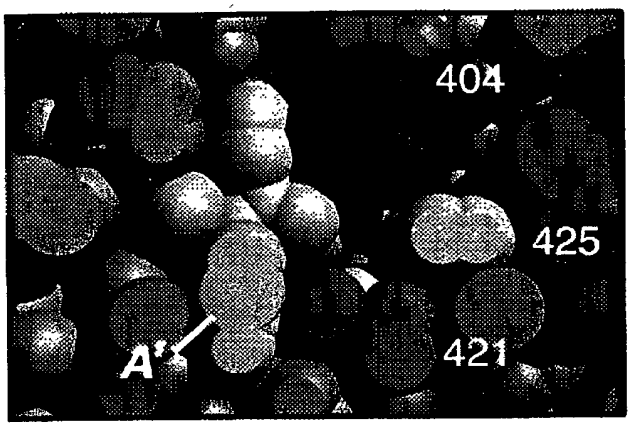
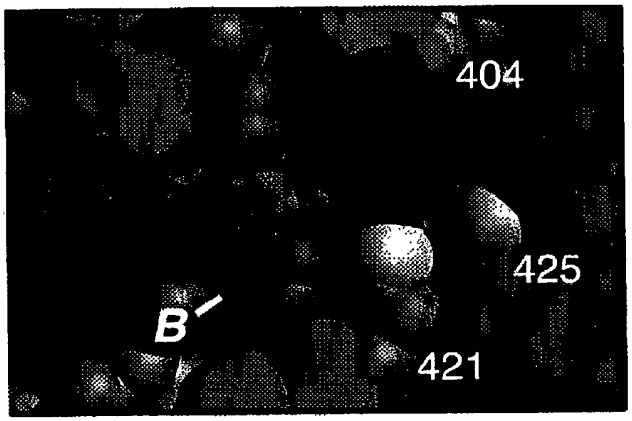


FIG._6C



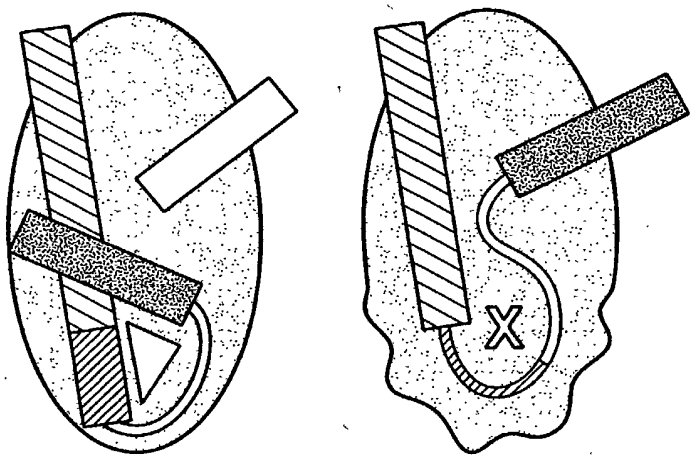


FIG._7

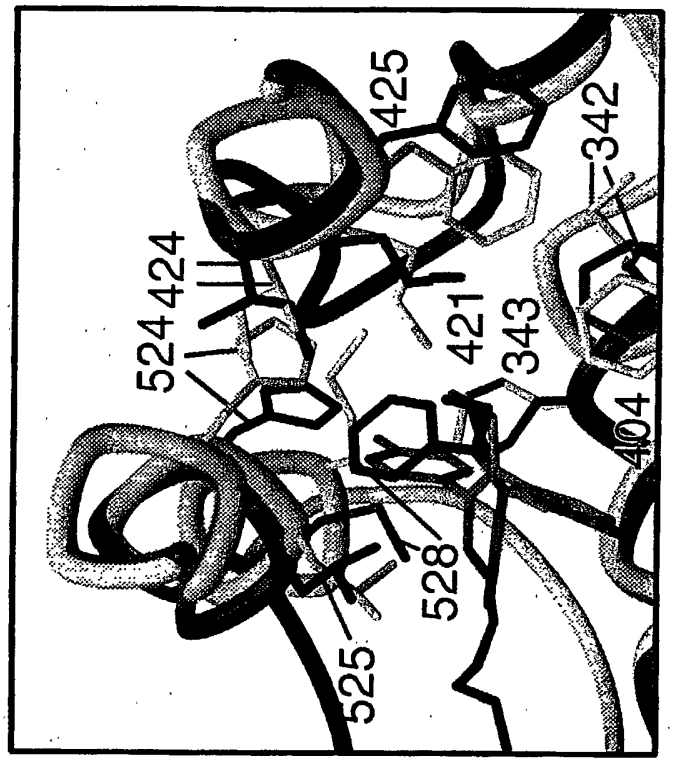


FIG._6D-2

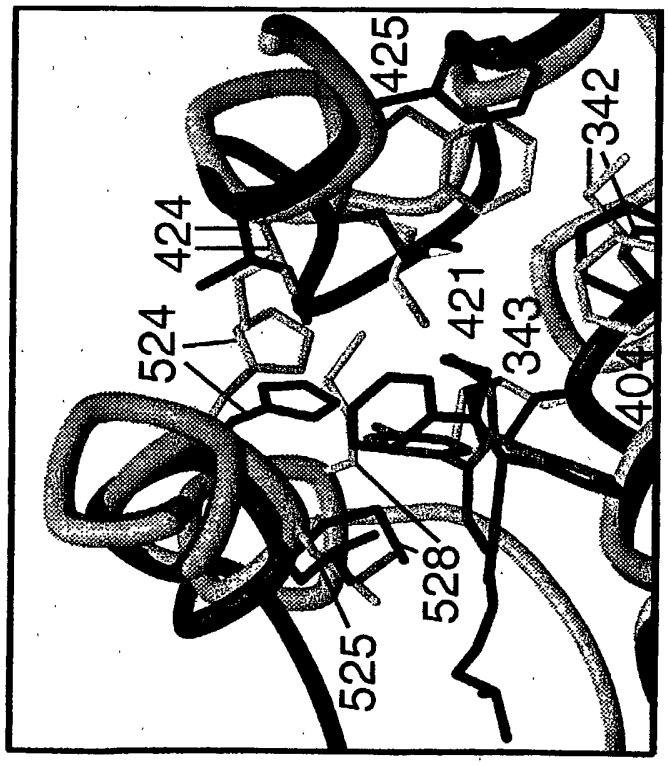


FIG._6D-1

		H3 (280 281 283 284 287 288)		H4 (293)		H5 (301 302 305 306)	H6 (309)			
hTRβ	277	TPAITRVVDFAK	KL	PMFC	ELP	CEDQIILLK	GCC	309	hTRβ	(SEQ ID NO:5)
rTRα	223	TPAITRVVDFAK	KL	PMFS	ELP	CEDQIILLK	CCC	255	rTRα	(SEQ ID NO:7)
hRARγ	235	TKCIIKIVEFAK	RL	PGFT	GLS	IADQITLLK	AAC	267	hRARγ	(SEQ ID NO:9)
hRXRα	273	DKQLFTLVEWAK	RI	PHFS	ELP	LDDQVILLR	AGW	305	hRXRα	(SEQ ID NO:11)
hPPARγ	288	VEAVQEITEYAK	NI	PGFI	NLD	LNDQVTLLK	YGV	320	hPPARγ	(SEQ ID NO:13)
hVDR	235	SYSIQKVIGFAK	MI	PGFR	DLT	SEDQIVLLK	SSA	267	hVDR	(SEQ ID NO:15)
hERα	351	DRELVHMINWAK	RV	PGFV	DLT	LHDQVHLLE	CAW	383	hERα	(SEQ ID NO:17)
hGR	568	GRQVIAAVKWAK	AI	PGFR	NLH	LDDQMTLLQ	YSW	600	hGR	(SEQ ID NO:19)
hPR	723	ERQLLSVVKWSK	SL	PGFR	NLH	IDDQITLIQ	YSW	755	hPR	(SEQ ID NO:21)
hMR	774	GKQMIQVVKWAK	VL	PGFK	NLP	LEDQITLIQ	YSW	806	hMR	(SEQ ID NO:23)
hAR	242	ERQLVHVVKWAK	AL	PGFR	NLH	VDDQMAVIQ	YSW	274	hAR	(SEQ ID NO:25)
		h hh hK		F		Qh hq	h			

FIG._8A

			H12 (453 454 457 458 459)			
hTRβ	450	LFP	PLFLEVF	ED	461	(SEQ ID NO:6)
rTRα	396	LFP	PLFLEVF	ED	407	(SEQ ID NO:8)
hRARγ	407	PMP	PLIREML	EN	418	(SEQ ID NO:10)
hRXRα	446	PID	TFLMEML	EA	457	(SEQ ID NO:12)
hPPARγ	462	SLH	PLLQEIY	KD	473	(SEQ ID NO:14)
hVDR	413	KLT	PLVLEVF	GN	424	(SEQ ID NO:16)
hERα	535	PLY	DLLLEML	DA	546	(SEQ ID NO:18)
hGR	748	EFP	EMLAEII	TN	759	(SEQ ID NO:20)
hPR	904	EFP	EMMSEVI	AA	915	(SEQ ID NO:22)
hMR	955	EFP	AMLVEII	SD	966	(SEQ ID NO:24)
hAR	423	DFP	EMMAEII	SV	444	(SEQ ID NO:26)
			h Eh			

FIG._8B

Attorney Docket No.: 407T-980510US
Client Reference No.: 99-016-2

DECLARATION

As a below named inventor, I declare that:

My residence, post office address and citizenship are as stated below next to my name; I believe I am the original, first and sole inventor (if only one name is listed below) or an original, first and joint inventor (if plural inventors are named below) of the subject matter which is claimed and for which a patent is sought on the invention entitled: **METHODS AND COMPOUNDS FOR MODULATING NUCLEAR RECEPTOR ACTIVITY** the specification of which __ is attached hereto or __x__ was filed on **March 30, 1999** as Application No. **09/830,693**.

I have reviewed and understand the contents of the above-identified specification, including the claims, as amended by any amendment referred to above. I acknowledge the duty to disclose information which is material to the examination of this application in accordance with Title 37, Code of Federal Regulations, Section 1.56. I claim foreign priority benefits under Title 35, United States Code, Section 119 of any foreign application(s) for patent or inventor's certificate listed below and have also identified below any foreign application for patent or inventor's certificate having a filing date before that of the application on which priority is claimed.

Prior Foreign Application(s)

Country	Application No.	Date of Filing	Priority Claimed Under 35 USC 119
WO	PCT/US99/50658	30 March 1999	

I hereby claim the benefit under Title 35, United States Code § 119(e) of any United States provisional application(s) listed below:

Application No.	Filing Date
60/079,956	March 30, 1998
60/113,146	December 16, 1998
60/113,014	December 16, 1998

I claim the benefit under Title 35, United States Code, Section 120 of any United States application(s) listed below and, insofar as the subject matter of each of the claims of this application is not disclosed in the prior United States application in the manner provided by the first paragraph of Title 35, United States Code, Section 112, I acknowledge the duty to disclose material information as defined in Title 37, Code of Federal Regulations, Section 1.56 which occurred between the filing date of the prior application and the national or PCT international filing date of this application:

Application No.	Date of Filing	Status

Attorney Docket No.: 407T-980510US
Client Reference No.: 99-016-2

Full Name of Inventor 1:	Full Name: **Andrew Shiau**		
Residence & Citizenship:	City: **San Francisco**	State/Foreign Country: **California** CA	Country of Citizenship: **US**
Post Office Address:	Post Office Address: **34 Hugo Street, Apt. ~~#13~~ #3 San Francisco, California 94122**		
Full Name of Inventor 2:	Full Name: **Peter J. Kushner**		
Residence & Citizenship:	City: **San Francisco**	State/Foreign Country: **California**	Country of Citizenship: **US**
Post Office Address:	Post Office Address: **1362 6th Avenue San Francisco, California 94122**		
Full Name of Inventor 3:	Full Name: **David A. Agard**		
Residence & Citizenship:	City: **San Francisco**	State/Foreign Country: **California**	Country of Citizenship: **US**
Post Office Address:	Post Office Address: **283 Juanita Way San Francisco, California 94127**		
Full Name of Inventor 4:	Full Name: **Geoffrey L. Greene**		
Residence & Citizenship:	City **Chicago**	State/Foreign Country: **Illinois**	Country of Citizenship: **US**
Post Office Address:	Post Office Address: **2020 Lincoln Park West, Apt. 25F Chicago, Illinois 60614**		

I further declare that all statements made herein of my own knowledge are true and that all statements made on information and belief are believed to be true; and further that these statements were made with the knowledge that willful false statements and the like so made are punishable by fine or imprisonment, or both, under Section 1001 of Title 18 of the United States Code, and that such willful false statements may jeopardize the validity of the application or any patent issuing thereon.

Signature of Inventor 1	Signature of Inventor 2	Signature of Inventor 3
Andrew Shiau	**Peter J. Kushner**	**David A. Agard**
Date NOVEMBER 30, 2001	Date	Date

declaration

Attorney Docket No.: 407T-980510US
Client Reference No.: 96-016-2

Full Name of Inventor 1	Full Name **Andrew Shiau**		
Residence & Citizenship:	City **San Francisco**	State/Foreign Country **California/The United States of America**	Country of Citizenship **US**
Post Office Address:	Post Office Address: **34 Hugo Street, Apt. #13** **San Francisco, California 94122**		
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Post Office Address:	Post Office Address **1362 6th Avenue** **San Francisco, California 94122**		
Full Name of Inventor 3:	Full Name: **David A. Agard**		
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Post Office Address:	Post Office Address: **283 Juanita Way** **San Francisco, California 94127**		
Full Name of Inventor 4:	Full Name: **Geoffrey L. Greene**		
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Post Office Address:	Post Office Address: **2020 Lincoln Park West, Apt. 25F** **Chicago, Illinois 60614**		

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Signature of Inventor 1	Signature of Inventor 2	Signature of Inventor 3
Andrew Shiau Date	**Peter J. Kushner** Date	**David A. Agard** Date

4-00

Signature of Inventor 4

Geoffrey L Greene

Geoffrey L. Greene 9/12/2001

Attorney Docket No.: 407T-980510US
Client Reference No.: 96-016-2

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Signature of Inventor 1	Signature of Inventor 2	Signature of Inventor 3
Andrew Shiau	**Peter J. Kushner**	**David A. Agard**
Date	Date	Date 9/12/01

Signature of Inventor 4
Geoffrey L. Greene

Attorney Docket No.: 407T-980510US
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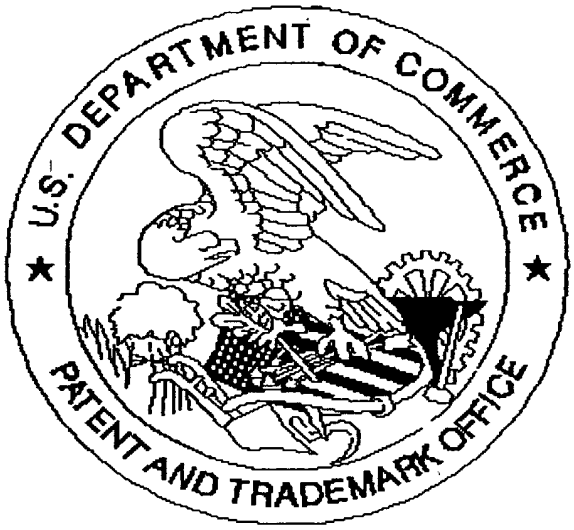
Signature of Inventor 1	Signature of Inventor 2	Signature of Inventor 3
Andrew Shiau	**Peter J. Kushner**	**David A. Agard**
Date	Date Sept 18, 2001	Date

Signature of Inventor 4
Geoffrey L. Greene

United States Patent & Trademark Office

Office of Initial Patent Examination -- Scanning Division



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